



**FisMat  
2015**



University of Palermo - September 28 - October 2, 2015 - Conference Chairs: Ezio Puppini (CNISM) - Corrado Spinella (CNR)

**Italian National Conference on  
Condensed Matter Physics  
(Including Optics, Photonics, Liquids, Soft Matter)**

*Palermo, September 28 - October 2, 2015*

**BOOK OF ABSTRACT**

**Editors**

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**UNIVERSITÀ  
DEGLI STUDI  
DI PALERMO**

Dipartimento di Fisica e Chimica



Dear colleagues,

it's a great pleasure for me to welcome all of you at FisMat 2015, the Italian conference on condensed matter physics and related fields. After the first edition in Milan two years ago this year the conference is held at the University of Palermo.

The first edition, after ten years, gathered the whole Italian community working in the field of condensed matter physics and related fields. The initiative demonstrated the relevance of organizing an event like this and the strong need to have such an inclusive meeting.

This year the conference takes place in Sicily, in the beautiful city of Palermo. It will be a great event as testified by the large number of oral contributions received, larger compared to the previous edition.

Ezio Puppini and Corrado Spinella (Conference Chairmen)

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# Plenary sessions

## Monday, September 28

- 11:00-12:00 **John Rogers** University of Illinois, Urbana Champaign (USA)  
“Semiconductor Nanomaterials for 3D Bioresorbable Electronics”
- 12:30-13:00 **Lydèric Bocquet** Ecole Normale Supérieure (France)  
“Flow and friction inside individual nanotubes: fast and curious”
- 17:00-18:00 **Michele Parrinello** ETH, Zurich (Switzerland)  
“Atomistic Modeling of Crystal Nucleation and Growth”

## Tuesday, September 29

- 09:00-10:00 **George Sawatzky** University of British Columbia (Canada)  
“Explicit role of O 2p states in high oxidation state (transition metal) Oxides”
- 14:00-15:00 **Alexei Ivlev** Max Planck Institute, Garching (Germany)  
“Two-dimensional complex plasmas: Equilibrium and non-equilibrium phenomena”
- 15:00-16:00 **Leo Kouwenhoven** QuTech, TUDelft (The Netherlands)  
“Experimental progress on Majoranas in semiconductors”

## Wednesday, September 30

- 09:00-10:00 **Daniel Shechtman** Technion, Haifa (Israel)  
“Quasiperiodic crystals: a paradigm shift in crystallography “
- 16:30-17:30 **Albert Polman** FOM Institute AMOLF, Amsterdam (The Netherlands)  
“Plasmonic optical metamaterials”

## Thursday, October 1

- 09:00-10:00 **Giorgio Parisi** Università “La Sapienza”, Rome (Italy)  
“On the physics of jamming”
- 17:30-18:00 **Enrico Gratton** University of California, Irvine (USA)  
“Chromatin structure and dynamics”

# Plenary lectures abstracts

## **Semiconductor Nanomaterials for 3D Bioresorbable Electronics**

John A. Rogers

*University of Illinois, Urbana Champaign (USA)*

Recent advances in semiconductor nanomaterials and deterministic assembly techniques enable the construction of high performance electronic and optoelectronic systems with 3D layouts and in bioresorbable forms. Potential applications range from temporary biomedical implants to active tissue scaffolds. This talk describes the key concepts in materials, physics and mechanics for (1) 3D mesoscale electronic networks as bio-interfaces, and (2) bioresorbable intracranial monitors and nerve stimulators.

## **Flow and friction inside individual nanotubes: fast and curious**

Lydéric Bocquet

*Laboratoire de Physique Statistique, Ecole Normale Supérieure*

Fluid transport at the nanoscales is one of the remaining virgin territory in fluid dynamics, in spite of hydrodynamics being a very old and established domain. A major challenge to address the fundamental properties at the nanoscales lies in building distinct and well-controlled nanosystems, amenable to the systematic exploration of their properties. To this end, we have developed new methods based on the manipulation of nano-objects, displacing, cutting, and glueing these elementary building blocks. This allows us to fabricate original fluidic and mechanical systems involving single (carbon and boron-nitride) nanotubes.

I will first discuss fluidic transport inside single nanotubes. Putting osmotic transport and its fundamental origins into perspective, I will show how to harvest this powerful mechanism beyond the classical van't Hoff law. Experiments of osmotic transport across boron-nitride show unprecedented energy conversion from salt concentration gradients. This points to new avenues in the field of osmotic energy harvesting from salinity gradient. These results will be then compared to those obtained with carbon nanotubes. They point to some key differences between these two materials which exhibit the same crystallography, but very different electronic properties.

Then I will explore the friction properties between the layers of boron-nitride and carbon nanotubes in a christmas-cracker geometry, in which a multiwalled nanotube is torn apart between a nanomanipulator and a quartz-tuning-fork-based atomic force microscope. We measure a huge viscous-like interlayer friction for BNNTs, whereas for the CNTs the sliding friction vanishes within experimental uncertainty. I will discuss possible mechanisms at the origin of the contrasting behaviors of CNTs and BNNTs.



## Atomistic Modeling of Crystal Nucleation and Growth

Michele Parrinello

*ETH Zurich, Department of Chemistry and Applied Sciences and Università della Svizzera italiana, Informatica, ICS, Via G.Buffi 13, 6904 Lugano, Switzerland*

Understanding crystal growth on nucleation is crucial for controlling crystal properties. Nucleation however takes place on a time scale that exceeds our ability to simulate this phenomena by straightforward atomistic molecular dynamics simulation. To this effect, we have developed metadynamics as very successful enhanced sampling method. We apply this approach to the study of nucleation from solution. We unveil the complex nature of this process and its deviation from standard theories. Finally, by taking advantage of recent development we are able to compute nucleation rates.

## Explicit role of O 2p states in high oxidation state (transition metal) Oxides

G.A.Sawatzky

*University of British Columbia*

For late 3d transition metal oxide with formally high oxidation states like  $\text{Cu}^{3+}$ ,  $\text{Ni}^{3+}$ ,  $\text{Co}^{4+}$ ,  $\text{Fe}^{4+}$ ,  $5+$ ,  $\text{Mn}^{4+}$ , and on a different but it turns out similar note  $\text{Bi}^{4+}$ , the charge transfer energy for transferring electrons from O to the transition metal may be negative resulting in a formally more correct starting point in which the oxidation state is lowered and holes in the O 2p orbitals are introduced. In this talk we present experimental evidence for this in a number of systems of present day importance and discuss the consequences in terms of magnetic properties and issues such as potential charge disproportionation. We use x ray spectroscopies and especially resonant inelastic x ray scattering (RIXS) and model cluster like calculations and variational approaches as well as density functional theory where applicable ( $\text{SrBiO}_3$ ) to demonstrate the importance of considering the hole occupation of the O 2p states explicitly and discuss some popular materials like the Cuprates, Nickelates, Cobaltates and  $\text{SrBiO}_3$ , from this rather different starting point. I will start with the cuprates and some new exact diagonalization and variational method calculations applicable for the cuprates including also the ARPES spectral function calculations. Here we demonstrate that it is of great importance to explicitly include the O 2p bands resulting in 3 spin polaron like quasiparticle states rather than the conventionally mostly used Zhang Rice singlet single band description. In this relatively new approach we can also explain the "effective" charge disproportionation observed with only very small actual charge motion as well as the charge and magnetic super lattice structure in the insulating rare earth Nickelates. We demonstrate that the low energy scale charge degrees of freedom are mainly of O 2p hole character with very strong electron phonon coupling forming O Octahedra molecular orbital like states in the low temperature phases. Recent RIXS results strongly support this negative charge transfer gap scenario. I will present arguments that actually these ideas are rather generally applicable to a very wide range of systems of compounds involving high cation oxidation states including systems like  $\text{Ba}(\text{Sr})\text{BiO}_3$  which when doped with K are fairly high temperature superconductors preceding the cuprate era.

## **Two-dimensional complex plasmas: Equilibrium and non-equilibrium phenomena**

Alexei Ivlev

*Max Planck Institute for Extraterrestrial Physics, Garching, Germany*

Complex plasmas are often employed as experimental model systems where charged microparticles play the role of “proxy atoms”. Two-dimensional (2D) complex plasmas, routinely obtained in laboratories, allow us to conduct particle-resolved studies of classical generic phenomena occurring in liquids and solids. In this talk I will summarize recent experimental and theoretical progress in investigating these systems.

I will start with the discussion of some generic mechanisms governing non-equilibrium melting and re-crystallization in 2D systems – such dynamical phenomena can be studied with 2D complex plasma at the individual-particle level. Furthermore, I will present the dominant plasma-specific mechanism of melting operating in 2D plasma crystals, the so-called “mode-coupling instability”, which is characterized by a well-defined threshold. The onset of the instability identifies the “dividing line” between the regimes where the melting is triggered by specific plasma processes, and where 2D complex plasmas act as a true model system.

Finally, I will focus on binary complex plasmas, where the interactions between different species can be made essentially nonreciprocal. This enables us to investigate general properties of various soft-matter systems where Newton’s third law is broken for the interparticle forces. In particular, we rigorously show that in certain cases such systems, being intrinsically non-equilibrium, can nevertheless be described in terms of equilibrium statistical mechanics and exhibit detailed balance with distinct temperatures for each species.

## **Experimental progress on Majoranas in semiconductors**

Leo Kouwenhoven

*QuTech, TUDelft, The Netherlands*

Majoranas in semiconductor nanowires can be probed via various electrical measurements. Tunnel spectroscopy reveals zero-bias peaks in the differential conductance. These zero-bias peaks have a particular dependence on magnetic field (amplitude and direction) and electron density. This dependence allows to falsify many alternative theories for the observations. New challenges include a direct demonstration of topological protection, which is provided by a parity protection: How stable is the system's occupation in terms of an even or an odd number of quasi-particles? We demonstrate that the quasi-particle parity in a superconducting Cooperpair box can be stable over timescales of minutes. To demonstrate this protection for Majoranas it is crucial that the induced superconducting gap has negligible sub-gap states. To obtain such hard gaps under Majorana conditions currently forms the most important challenge. We report on progress in optimizing materials and measurement techniques.

## Quasi-periodic crystals – a paradigm shift in crystallography

D. Shechtman

*Technion, Haifa, Israel and ISU, Ames, Iowa, USA*

Crystallography has been one of the mature sciences. Over the years, the modern science of crystallography that started by experimenting with x-ray diffraction from crystals in 1912, has developed a major paradigm – that all crystals are ordered and periodic. Indeed, this was the basis for the definition of “crystal” in textbooks of crystallography and x-ray diffraction. Based upon a vast number of experimental data, constantly improving research tools, and deepening theoretical understanding of the structure of crystalline materials no revolution was anticipated in our understanding the atomic order of solids.

However, such revolution did happen with the discovery of the Icosahedral phase, the first quasi-periodic crystal (QC) in 1982, and its announcement in 1984 [1, 2]. QCs are ordered materials, but their atomic order is quasiperiodic rather than periodic, enabling formation of crystal symmetries, such as icosahedral symmetry, which cannot exist in periodic materials. The discovery created deep cracks in this paradigm, but the acceptance by the crystallographers' community of the new class of ordered crystals did not happen in one day. In fact it took almost a decade for QC order to be accepted by most crystallographers. The official stamp of approval came in a form of a new definition of “Crystal” by the International Union of Crystallographers. The paradigm that all crystals are periodic has thus been changed. It is clear now that although most crystals are ordered and periodic, a good number of them are ordered and quasi-periodic.

While believers and nonbelievers were debating, a large volume of experimental and theoretical studies was published, a result of a relentless effort of many groups around the world. Quasi-periodic materials have developed into an exciting interdisciplinary science.

This talk will outline the discovery of QCs and describe the important role of electron microscopy as an enabling discovery tool.

[1] D. Shechtman, I. Blech, *Met. Trans.* 16A (June 1985) 1005-1012.

[2] D. Shechtman, I. Blech, D. Gratias, J.W. Cahn, *Phys. Rev. Letters*, Vol 53, No. 20 (1984) 1951-1953.

## Plasmonic optical metamaterials

Albert Polman

*Center for Nanophotonics, FOM Institute AMOLF, Amsterdam, The Netherlands*

Optical metamaterials are materials with a subwavelength architecture that have optical properties that do not exist in natural materials. We present metallo-dielectric metamaterials, based on 2D and 3D nanoscale assemblies of noble metals and dielectrics that show a negative refractive index. These unusual characteristics are used to realize a flat lens with unique features such as a submicron thickness, the absence of an optical axis and a lens-image separation of only 350 nm. The image is formed by the coherent superposition of negatively refracted light from multiple harmonics in the metamaterial. Metallodielectric nanostructures can also serve as transparent contacts on solar cells, as we will demonstrate. Finally, we demonstrate a new thermodynamically driven plasmoelectric effect that generates a photovoltage under off-resonant excitation of a plasmonic metasurface.

## **On the physics of jamming**

Giorgio Parisi

*Università di Roma “La Sapienza”*

Jamming is a well known phenomenon that you have experienced when the traffic is very heavy. You cannot move because your neighbors block you and your neighbors cannot move because you block them. Jamming is a collective phenomenon. Marble pebbles on the beach are one example of jamming. However also for well-leveled pebbles, friction will play an important role.

Equilibrium statistical mechanics may be used to study the case of systems without friction. The most studied case is the hard sphere gas where the jamming point is reached in the limit of infinite pressure. In the case of frictionless jamming long-range correlations are present: we have a new kind of critical system.

Recently the properties of the hard sphere gas have been analytically computed in the framework of the mean field approximation. Non-trivial critical exponents have been found. The behavior of the correlation functions at large distances has not yet been computed (it is technically very challenging): at the end one should find a new scaling invariant field theory.

## **Chromatin structure and dynamics**

Enrico Gratton and Paolo Annibale

*Laboratory for Fluorescence Dynamics, Department of Biomedical Engineering, University of California, Irvine*

Chromatin structure, compaction and remodeling at the micro and nanometer scale have fundamental roles in many biological events. Chromatin compaction produces heterogeneity of the cell nucleus which results in structural and transport properties which have been only partially studied. Although the nucleosome structure has been in part deciphered, the topology of chromatin structure at the micron scale remains unresolved. In this work, we studied chromatin organization using the orbital 3D tracking technique. This method provides insight of local structure and transport properties at the nano scale by following the trajectories of molecules during gene expression.

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# Parallel sessions

## **28 Sept - PM**

Computational Biophysics I  
Cultural Heritage  
Simulations of Materials for ICT  
Plasma Physics I  
Magnetism and spin related phenomena I  
Cuprates and Mechanisms for Superconductivity 28 Sept  
Optical feedback and metamaterials in mid-IR and THz  
Sustainable Nanotechnologies I  
Nanophotonics I  
Laser-Matter Interaction: from Atoms to Nano-Particles

## **29 Sept - AM**

Computational Biophysics II  
Interdisciplinary statistical physics  
From nanoparticles to nanostructured surfaces  
Plasma Physics II  
Magnetism and Spin related phenomena II  
Iron Based Superconductors  
Oxide Films and Interfaces  
Sustainable Nanotechnologies II  
Quantum Fluctuations and Casimir Forces  
2D emerging materials I  
Nanophotonics II  
THz and Quantum Cascade Lasers

## **29 sep - PM**

Computational Biophysics III  
Diffusion and reaction in complex systems  
Noncovalent interactions: advances in Computer Simulations  
Plasma Physics III  
Magnetism and Spin related phenomena IV  
Optical bio-sensing  
3d and 5d TM systems  
Sustainable Nanotechnologies III  
Photovoltaic materials and devices  
2D emerging materials II  
Optofluidics

## **30 Sept - AM**

Molecular Biophysics I

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Statistical Mechanics of Active Matter  
Light Manipulation  
Plasma Physics IV  
Magnetism and Spin related Phenomena III  
Thin films, Devices, Weak Superconductivity and Applications  
Topological Insulators  
Non Linear Optics  
Photonic and plasmonic materials and devices

### **1 Oct - AM**

Biophysical Models I  
Correlated electrons and cold atoms  
Imaging and non-destructive analysis  
New physics with ultrashort light and x-ray pulses I  
Quantum Optics and Coherent Manipulation  
Organic on Substrates I  
Gas Sensors and Biosensors for Health and Wealth  
Advanced Optical Materials I  
Electronic and optical properties of low dimensional systems I  
Soft Matter I 1 Oct  
Advanced materials for energy applications I

### **1 Oct - PM**

Biophysical Models II  
Transport and anomalous dynamics  
Molecular liquids in equilibrium and non-equilibrium regimes  
Geophysics  
New physics with ultrashort light and x-ray pulses II  
Quantum thermodynamics and quantum technologies 1  
Organic on Substrates II  
Nanomaterials and Nanotechnology: carbon nanotubes  
Advanced Optical Materials II  
Electronic and optical properties of low dimensional systems II  
Soft Matter II 1 Oct  
Advanced materials for energy applications II

### **2 Oct - AM**

Advanced Microscopy Techniques  
Out of Equilibrium Statistical Mechanics I  
Econophysics  
Environmental Physics and Pollution  
Dosimetry  
Quantum thermodynamics and quantum technologies 2  
Diamond-based substrates and Memristors for Brain sensing  
Metrology  
Fiber and Miniaturized Optical Sensors  
Electronical and optical properties of low dimensional systems III

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Synchrotron radiation and material science I  
Advanced materials for energy applications III

**2 Oct - PM**

Molecular Biophysics II  
Out of Equilibrium Statistical Mechanics II  
Complex Networks in Economy, Biology, ...  
Physical Processes in Volcanic Eruptions  
Biomedical Applications  
Complexity in the brain  
Nanomaterials and Nanotechnology: Graphene  
Advanced optical characterization techniques  
Synchrotron radiation and material science II

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# September 28

<b>Computational Biophysics I</b>	<b>Leonardo Guidoni</b>
<b>Cultural Heritage</b>	<b>Maria Brai</b>
<b>Simulations of Materials for ICT</b>	<b>Riccardo Ferrando</b>
<b>Plasma Physics I</b>	<b>Stefano Atzeni</b>
<b>Magnetism and spin related phenomena I</b>	<b>Riccardo Bertacco</b>
<b>Cuprates and Mechanisms for Superconductivity</b>	<b>Giacomo Ghiringhelli</b>
<b>Optical feedback and metamaterials in mid-IR and THz</b>	<b>Sukhdeep Dillon</b>
<b>Sustainable Nanotechnologies I</b>	<b>Stefania Milioto</b>
<b>Nanophotonics I</b>	<b>Miriam Vitiello</b>
<b>Laser – Matter Interaction: from Atoms to Nano - Particles</b>	<b>Emilio Fiordilino</b>



**#001 - Computational approaches to RNA unzipping dynamics**

*Giovanni Bussi (I) - Scuola Internazionale Superiore di Studi Avanzati*

RNA is acquiring a large importance in cell biology, as more functions that it accomplishes are discovered. However, experimental characterization of RNAs dynamical behavior at atomistic level is difficult. Explicit solvent and structure based molecular dynamics, in combination with state-of-the-art free-energy techniques and advanced analysis protocols, can bridge the gap providing an unparalleled perspective on the mechanism and dynamics of RNA folding and conformational transitions.

In this talk I will give an overview of our applications on the intrinsic and helicase-dependent RNA unzipping dynamics. I will discuss a model for RNA unzipping that reconciles otherwise puzzling biochemical data and offers an intuitive understanding of the mechanisms underlying the directionality of helicases [1,2]. Moreover, I will show how explicit solvent molecular dynamics in combination with enhanced sampling techniques can be used to characterize the translocation intermediates of a prototypical RNA helicase [3].

[1] Colizzi and Bussi, *J. Am. Chem. Soc.* 134, 5173 (2012)

[2] Colizzi and Bussi, Asymmetric double helix opening drives helicases unwinding dynamics, submitted (2015)

[3] Perez-Villa, Darvas, and Bussi, *Nucleic Acids Res.* doi: 10.1093/nar/gkv872 (2015)

**#002 - Computational studies on efflux pumps of the RND superfamily**

*Paolo Ruggerone (I) - University of Cagliari*

*Other Authors: Attilio V. Vargiu (Department of Physics, University of Cagliari, Cittadella Universitaria, S.P. Monserrato-Sestu km 0.700, I-09042 Monserrato (CA), Italy), Pierpaolo Cacciotto (Department of Physics, University of Cagliari, Cittadella Universitaria, S.P. Monserrato-Sestu km 0.700, I-09042 Monserrato (CA), Italy)*

In this talk I will give a summary of the work performed in our group on the efflux pumps AcrAB-TolC of *E. coli* and MexAB-OprM of *P. aeruginosa*, including recent unpublished data. The first part will focus on the RND transporters MexB and AcrB, namely on the mechanisms of uptake, recognition and extrusion of substrates by this protein. The second part will focus on assessing the role of MexA multimerization for the assembly of the MexAB-OprM pump.

**#003 - Molecular dynamics (MD) study of the human adenosine receptor type 2A in complex with caffeine**

*Giulia Rossetti - IAS-5/INM-9: Computational Biomedicine - Institute for Advanced Simulation (IAS)/Institute of Neuroscience and Medicine (INM)*

*Other Authors: Ruyin Cao (1), Andreas Bauer (2), Paolo Carloni (1, 2) (1) German Research School for Simulation Sciences (joint venture of RWTH Aachen University and Forschungszentrum Jülich), D-52425 Jülich, Germany and Computational Biomedicine, Institute for Advanced Simulation (IAS-5), Forschungszentrum Jülich, D-52425 Jülich, Germany (2) Institute of Neuroscience and Medicine (INM-9), Forschungszentrum Jülich, D-52425 Jülich, Germany*

Lipid composition may significantly affect membrane proteins function, yet its impact on the protein structural determinants is not well understood. Here we present a comparative molecular dynamics (MD) study of the human adenosine receptor type 2A (hA<sub>2A</sub>R) in complex with caffeine – a system of high neuro-pharmacological relevance – within different membrane types. These are POPC, mixed POPC/POPE and cholesterol-rich membranes. 0.8- $\mu$ s MD simulations unambiguously show that the helical folding of the amphipathic helix 8 depends on membrane contents. Most importantly, the distinct cholesterol binding into the cleft between helix 1 and 2 stabilizes a specific caffeine binding pose against others visited during the simulation. Hence, cholesterol presence (~33%-50% in synaptic membrane in central nervous system), often neglected in X-ray determination of membrane proteins, affects the population of the ligand binding poses. We conclude that including a correct description of neuronal membranes may be very important for computer-aided design of ligands targeting hA<sub>2A</sub>R and possibly other GPCRs.

**#004 - Bitter taste perception: Insights from multiscale computational approaches**

*Alejandro Giorgetti - Dept. of Biochemistry, University of Verona*

Bitter taste perception: Insights from multiscale computational approaches

Giorgetti, Alejandro

*Department of Biotechnology, University of Verona, Verona, Italy and Computational Biophysics, German Research School for Simulation Sciences, Juelich, Germany*

Sensing chemicals present in the food is of fundamental importance for the survival of the species. Life evolved a host of mechanisms to communicate chemical information from the environment to elicit cellular responses that provide an advantage in avoiding or seeking the chemical signatures of foods, mates, toxins, etc. In particular, mammals during evolution have been prevented from ingesting toxic compounds because of their strong bitter taste. This protection mechanism has been carried out by a family of 25 bitter taste receptors (TAS2Rs). A characterization of the mechanisms underlying their function is lacking. Here I will present our studies on the interaction of TAS2R38 with two of its agonists. Indeed, by using a combination of homology models together with docking, molecular mechanics/coarse-grained (MM/CG) simulations and experimental data, we were able to provide a detailed description of the ligand-binding site in the receptors, satisfying site-directed mutagenesis experiments. Our approach could be used for other GPCRs with direct applications in drug design.

#### **#005 - Multiscale molecular simulations to investigate pharmaceutically relevant metalloenzymes**

*Marco De Vivo - Laboratory of Molecular Modeling and Drug Discovery - Istituto Italiano di Tecnologia*

Multiscale molecular simulations, covering broad temporal and spatial scales, is critical for understanding both physical and chemical steps of enzymatic catalysis and disclose mechanistic insights potentially useful for designing better drugs. Here, I will present a few representative examples where multiscale molecular simulations based on classical molecular dynamics (MD) coupled with quantum mechanics/molecular mechanics (QM/MM) simulations have been used to investigate enzymes that are important targets for drug discovery. In particular, I will focus on MD and QM/MM studies that address the role of catalytic metal ions for enzymatic processing of DNA and RNA. Ultimately, through a series of examples, I aim to demonstrate that multiscale simulations is an effective means to envision and dissect new mechanistic hypotheses that involve a larger and more flexible metal-centered structural architecture in important metalloenzymes. Although the impact of MD and QM/MM simulations on practical drug discovery is still limited, these once prohibitive methods for effective drug design are now increasingly used for structure-based discovery. Findings from these studies, for example, might be of practical interest for the design of potent inhibitors that resemble the enzymatic transition state.

#### **#006 - A database of force-field parameters, dynamics, and properties of antimicrobial compounds**

*Giuliano Mallocci - Department of Physics - University of Cagliari*

*Other Authors: Attilio Vittorio Vargiu (Department of Physics - University of Cagliari), Giovanni Serra (Department of Physics - University of Cagliari), Andrea Bosin (Department of Physics - University of Cagliari), Paolo Ruggerone (Department of Physics - University of Cagliari), Matteo Ceccarelli (Department of Physics - University of Cagliari)*

We present an on-line database of all-atom force-field parameters and molecular properties of compounds with antimicrobial activity (mostly antibiotics and some beta-lactamase inhibitors). For each compound, we provide the General Amber Force Field parameters for the major species at physiological pH, together with an analysis of properties of interest as extracted from microsecond-long molecular dynamics simulations in water and counter ions. The properties include number and population of structural clusters, molecular flexibility, hydrophobic and hydrophilic molecular surfaces, the statistics of intra- and inter-molecular H-bonds, as well as structural and dynamical properties of solvent molecules within first and second solvation shells. In addition, the database contains several key molecular parameters, such as energy of the frontier molecular orbitals, vibrational properties, rotational constants, atomic partial charges and electric dipole moment, computed by Density Functional Theory. The present database (to our knowledge the first extensive one including dynamical properties) is part of a wider project aiming to build-up a database containing structural, physico-chemical and dynamical properties of medicinal compounds using different force-field parameters with increasing level of complexity and reliability.

#### **#007 - Local electric field in general porins of Gram-negative bacteria from all-atom simulations**

*Igor Bodrenko - Department of Physics, University of Cagliari*

*Other Authors: S. Acosta Gutierrez (Department of Physics, University of Cagliari, Italy), M.A. Scorciapino (Department of Biomedical Sciences, University of Cagliari, Italy; Istituto Officina dei Materiali del Consiglio Nazionale delle Ricerche (IOM-CNR), UOS, Cagliari, Italy), M. Ceccarelli (Department of Physics, University of Cagliari, Italy; Istituto Officina dei Materiali del Consiglio Nazionale delle Ricerche (IOM-CNR), UOS, Cagliari, Italy)*

Non-specific water-filled protein channels (porins) modulate the passive diffusion of nutrients in the outer membrane of Gram-negative bacteria. Also, polar antibiotics enter through this pathway and down-regulation and/or mutation of porins are very common in drug resistant strains. The profile of the local electric field along the channel together with the channel cross section profile play the key role in the translocation mechanism of polar molecules through a porin and in the filtering of molecules by porins.

We present a computational protocol to determine the local electric field in a porin by analyzing the ordering of water molecules inside the channel in the course of an all-atom molecular dynamics simulation.

In the application of the method to the OmpC porins from a series of clinical strains of *E.coli*, we demonstrate a significant change of the electric field profile in the antibiotic-resistant mutations while the channel cross section profile is well conserved within the series of the porins. Thus, the mutation leading to the specific modification of the local electric field on the porin is one of the mechanisms of developing resistance to antibiotics by suppressing their penetration into the bacteria.



**#008 - New perspectives in luminescence dating**

*Marco Martini (I) - Università di Milano-Bicocca*

In recent years, the application of physical techniques to the Cultural Heritage has experienced extraordinary developments and improvements, due to the wide spectrum of available scientific methodologies which support the traditional philological approach. Specifically looking at chronological aspects, most of the materials found on the field or in architectural structures can now be dated, or at least useful chronological indications can be reached, by the use of scientific techniques: in fact, besides radiocarbon mass spectrometry ( $^{14}\text{C}$ -AMS), used for organic materials, thermoluminescence (TL) and optically stimulated luminescence (OSL) are used to date ceramics and bricks. However, uncertainties in the interpretation of the results still exist. For example, the routine TL dating technique is widely used to assess specific chronologies to parts of a building, in order to assess construction sequences, and eventually to highlight restoration and modern remakes. However the obtained date refers to the making of the bricks rather than to the building construction. New perspectives toward the solution of such ambiguities are coming from techniques developed for the study of mortar and from the possibility of surface dating. This last is based on the OSL signal, which is bleached by the last exposure to sunlight. The same principle has been exploited in order to date the last exposure to the light of stone artifacts.

The main troubles derive from the evaluation of the initial erasure of the accumulated OSL signal, which is generally bleached with more than a single mechanism. An accurate study of the interaction of light with electron levels in the material is a fundamental requirement for understanding the bleaching process which is the basis of the application. Preliminary results on OSL dating of brick samples will be presented.

**#009 - Scientific and technical assistance in cultural heritage restoration projects**

*Monica Alvarez de Buergo (I) - Instituto de Geociencias IGEO (CSIC, UCM)*

Several real case studies will be shown in which scientific and technical assistance has been definitive and essential to plan conservation-restoration interventions, before, during and after the projects execution, as well as some recommendations for an effective preventive conservation.

The combination of traditional or laboratory techniques and equipments together with non destructive and portable techniques results very effective and helpful for the knowledge of the properties of cultural materials, the diagnosis (causes and processes of decay) and the assessment of the best, most adequate, effective and suitable conservation and restoration techniques and methods, with the possibility of monitoring the interventions in a short and medium term. Monitoring of environmental conditions are also considered to provide the clue of many decay processes

In the examples of cultural heritage in which scientific knowledge contributed to its conservation and restoration, the methodology followed and the techniques used for will be shown, such as for assessing the best cleaning method - and what is necessary to be removed and what not -, how to evaluate consolidant and hydrophobing products in each case, if the desalination method to be used to removing salts is efficient or not, if the raw materials that are to be used for restoration materials are the adequate or not, to locate the original quarries from which the element or structure was used, etc.

Examples from all over the world will be shown in a variety of building materials used in buildings, sculptures and archaeological sites, trying to transfer the methodology that the research group Petrology Applied to Heritage performs, together with the Petrophysics Laboratory, a laboratory coordinated by the group and one of the most specialized in cultural heritage research.

A review of the standardization in cultural heritage will be also done, together with the most relevant scientific reviews in stone conservation.

Last, but not least, the importance in transferring this scientific and technical knowledge to the society will be exposed.

**#010 - Elemental, molecular mapping and reflectance imaging for the characterisation of paintings**

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We propose a completely non-invasive approach based on the combination of different imaging techniques: X-Ray Fluorescence (XRF) mapping, Raman mapping, visible multispectral imaging and near-infrared (NIR) reflectography, aimed at identifying and mapping pigments in paintings. XRF mapping is performed through a new portable scanning device developed by XGLab SRL. The compact XRF head is driven by two light linear motors. The excitation, which is not guided by any X-ray optics, allows the acquisition of the fluorescence spectrum emitted with a good sensitivity also to lighter elements. The maximum scan-area depends on the tripod and motor arrangements, with typical values of  $10\text{ cm}^2$ . The remote Raman spectrometer is a custom-made transportable system based on a 785 nm diode laser, a pair of galvanometric mirrors and a custom optical system. The device can easily map a surface of 9 cm in diameter at a working distance of 30 cm. It is also possible to acquire Raman spectra of a single point of interest with a standard diffusive micro-probe at a shorter working distance of about 5 mm, and can reach the inelastic scattered signal with higher spatial and spectra resolution. The two complementary mapping techniques allow the acquisition of

elemental and molecular data, providing pigment identification with a high degree of confidence. Moreover, XRF spectra can allow the mapping of the sub-layer distribution of elements complementing data regarding the presence of hidden painted layers provided by NIR-reflectography. In the proposed approach, visible multispectral imaging, combined with novel methods of cluster analysis of multivariate spectral data makes it possible to map areas of paintings with similar spectral features and color properties, which correlate with the presence of the same pigment or mixture of pigments. Examples of applications on model paintings and in situ case studies will be discussed. In particular in-situ analysis on two 15-16th C illuminated manuscripts highlight the approach in the characterization of the color palette the detection of hidden paint layers and anachronistic pigments, which yielded valuable information for identifying the original owners and the history and trade of the artworks. Advantages of this image-based multi-analytical approach will be discussed, thus informing future analysis on other heterogeneous works of art.

#### #011 - LIBS analysis for a stratigraphic study on Cultural Heritage materials

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Among the possible analytical approaches for Cultural Heritage studies, the Laser-Induced Breakdown Spectroscopy (LIBS) allows deep profile analysis with high spatial resolution enough to discriminate different layers in the typical complex structures [1, 2].

LIBS, based on the principles of laser ablation, allows a detailed stratigraphic analysis on the basis of spectra recorded from successive laser pulses delivered onto the same sample point. This technique has significant advantages, even if the assessment of potentialities in the quantitative analyses are object of several works. It is well-known that performance of LIBS in qualitative and quantitative analysis is affected by many factors related to plasma formation and evolution, still now under investigation.

The aim of this work is to show the importance of finding the optimum parameters for different material typologies in order to acquire the maximum information with the least damage to the works of art.

The results concern mainly the comparison between the identification of the chemical elements by using the more traditional X-Ray fluorescence technique and the study of their distribution along the thicknesses of the layers from the Laser-Induced Breakdown Spectroscopy analyses.

The collected data have demonstrated the usefulness of the Laser-Induced Breakdown Spectroscopy investigation, through which it has been possible to reveal chemical elements undetectable by X-ray Fluorescence spectroscopy [3, 4], and to analyse the stratigraphic sequence of archaeological corroded bronzes, salt efflorescence on mural paintings and paint layers from the surface up to the bulk.

This methodological approach through the LIBS analysis, although micro - destructive, avoids the sampling, allowing a stratigraphic analysis with high spatial resolution and accuracy of the sample point localization.

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#### #012 - XRF and LIBS integrated analysis to identify the chemical composition and the conservation state of photographic and paper materials

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In the early period, even though professional photographers worked with similar techniques and products, their artistic and commercial aims determined different choices and lead them to follow different, often personal, recipes. For this reason, identification of the techniques through date and name of the photographer or some visual features like colour, tonality and

surface of the image layer, often needs further investigation to be proved. Chemical characterization, carried out in a non-invasive way, can be crucial to provide useful information about original composition, degradation process, realisation technique and conservative treatments. In this case, X Ray Fluorescence (XRF) analysis was used to confirm the chemical composition of eleven historical photographs (nine silver gelatine prints and two albumen prints) dated between the end of the 19th century and the beginning of the 20th, shot in Palermo (Sicily) by a popular photographer of the time, and pasted on their original cardboards. The elemental identification showing important information on different photographic realization techniques in terms of distribution of main chemical elements in the photographic film. Inappropriate storage caused severe degradation on both the prints and the backing boards that show physical, biological and chemical damages. An integrated approach based on XRF and Laser Breakdown Spectroscopy (LIBS) allowed to verify the spatial distribution of constituting chemical element on a typical chromatic alteration of paper, the so called *foxing*, a quite complex phenomenon, not yet well understood, which deserves further investigation. In particular, the variation of calcium and iron peak intensity signal from not degraded paper to *foxing* stains center has been monitored.

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### #013 - Use of holographic projections for the fruition and valorisation of cultural heritage

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In recent years is growing the interest in using multimedia supports to enhance the communication and educational aspect in the museums. The unique feature of Digital Holography in creating real 3D images, pave a way towards the future. Applications of holography to museum practice seem to be rather promising. Holographic methods may be a means capable of appreciably raising and improving the state of technical equipment of present-day museums, being able to create "real 3D" images. Nowadays, in a number of museums, are presented projections incorrectly labeled as "holographic", being instead 2D images displayed onto special semitransparent screens. To achieve real 3D-display, the emerging digital holography techniques offer new perspectives for future museum applications, in combination with multimedia systems.

The Istituto di Scienze Applicate e Sistemi Intelligenti has been active obtaining valuable results in registration, numerical elaboration and optical reconstruction of digital holograms, as well as in developing a new method for Infrared Digital Holography. The latter allows for very noticeable results in recording holographic images of large sized objects (up to human height) thus overcoming the previous limits. The holograms are recorded by a CCD camera, stored by a PC and sent to a Spatial Light Modulator (SLM), a special micro-device capable to display holograms at high frame rate allowing for holographic dynamic scene. In this case, a sequence of holograms was acquired, by using Infrared light. The SLM performs a fast sequence of optical reconstructions of them, with visible light.

The possibility of numerical handling holograms allows for any type of image elaboration on single holograms: changes in size and/or position in the space of the holographic reconstructed images, changes of focus plane, etc. The ability to merge distinct holograms of individual objects, each numerically elaborated, allows for optical projection of 3D holographic dynamic sequences. Modern museum tasks include not only conservation and preservation of material items, but also educational activities, implemented by using a number of multimedia systems. We showed how digital holography, for display use, could play an important role in this field, thanks to its unique ability in generating "Real 3D" scenes. Some results of current researches at Istituto di Scienze Applicate e Sistemi Intelligenti They will be presented.

### #014 - RADIOCARBON DATING OF MORTAR

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The carbon dioxide contributing to binder formation during the set of a lime mortar reflects the atmospheric  $^{14}\text{C}$  content at the time of construction of a building. For this reason, the  $^{14}\text{C}$  dating of mortars is used with increasing frequencies in archaeological and architectural research. Mortars, however, may also contain carbonaceous contaminants potentially affecting radiocarbon dating.

Recently has been obtained some promising results in mortar radiocarbon dating, thanks to the development of a procedure (i.e. CryoSonic/Cryo2Sonic) aiming to eliminate exogenous C contamination that may occur in a mortar. In particular a novel physical pre-treatment for the isolation of the atmospheric  $^{14}\text{CO}_2$  signal absorbed by the mortars during their setting, has been proposed. The protocol allows suppression of the fossil carbon (C) contamination originating from the incomplete burning of the limestone during the quick lime (CaO) production, providing unbiased dating for the mortar or lime lumps contained in the mortar. Moreover, a detailed petrographic characterization of mortars was used both as a preliminary tool for the choice of samples and to infer about the lack of accuracy (when verified) of the applied mortar  $^{14}\text{C}$  dating procedure.

In the present talk, we present AMS Radiocarbon dates performed on lime lumps with the aim to:

i) verify procedure accuracy by a comparison of the results obtainable from lime lumps dated after different treatments (i.e. bulk lime lumps vs CryoSonic purified lime lumps);

ii) compare different building phases absolute chronology for the medieval UNESCO site of Modena, with that assumed by historical sources in order to assess preliminary the  $^{14}\text{C}$  dating feasibility for of the site.

**#015 - Colour degradation of artwork: An ab initio study of the adsorption of oxygen and water on the surface of CdS pigment**

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The cadmium yellow paints (CdS) used in impressionist and modernist paintings in early 1900s are undergoing several deterioration processes whitening and discoloration. This discolored crusts at the surface of the paintings is formed mainly by white globular hydrated cadmium sulfate ( $\text{CdSO}_4 \cdot n\text{H}_2\text{O}$ ) and cadmium carbonate ( $\text{CdCO}_3$ ). The input for the formation of such whitish compounds is generally ascribed to an initial photo-oxidation process of Cd-yellow or to products used during the syntheses of CdS. [1,2]. Also, structural defects in CdS (deep traps) may play a role in the pigment alteration process [3].

In order to understand the oxidation and hydration mechanisms of the whitish globules, at atomic level, we present a theoretical study of points defects, namely Cd- and S- vacancies, both in the bulk and in the hexagonal non-polar {10.0} surface. The interaction between the {10.0} defective surface of CdS and  $\text{O}_2$  and  $\text{H}_2\text{O}$  molecules is then studied to simulate the combined effects of exposure to air and humidity. To this end the surface of CdS containing Cd- and S- vacancies was simulated according to the slab geometry and was next covered by oxygen, a water molecule and a combination of  $\text{O}_2 + \text{H}_2\text{O}$ . More specifically, we determined the favorite adsorption sites and calculated the adsorption energies of the different molecules on top of the surface. The details of the electronic structure of the interactions are given via the bonding charge analysis along with a thorough description of the geometry. Also, For this purpose, we adopted a first principles method within the framework of the Density Functional Theory (DFT) in the Generalized Gradient Approximation (GGA-PBE) with the use of ultrasoft pseudopotentials as implemented in the quantum-ESPRESSO package [4].

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**#016 - Exotisms in layered perovskites: multiferroics, magnetoelectrics and a ferroelectric metal**

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Just as their standard counterpart, layered perovskite are emerging as an interesting player in the field of multiferroicity and beyond. I will discuss examples of exotic behavior in the family  $A_nX_nO_{3n+2}$ , and showcase the first known native ferroelectric metal,  $Bi_5Ti_5O_{17}$ , exhibiting the coexistence of metallicity and spontaneous polarization, as well as (with some tweaking) depolarizing fields in a finite system. Time permitting, I will address the insulating  $n=4$  case, where the highlights are the weak ferromagnet  $La_2Mn_2O_7$  with its anomalously large linear magnetoelectric coupling, and V-doped  $La_2Ti_2O_7$ , a ferroelectric ferromagnet exhibiting the quintessential magnetoelectric effect, i.e. magnetization inversion upon polarization inversion.

**#017 - Atomistic simulations of phase change materials for non-volatile memories**

Marco Bernasconi (I) - University of Milano-Bicocca

Chalcogenide phase change alloys are attracting an increasing interest because of their use in optical digital versatile disc, DVD and electronic (phase change memories, PCM) data storage devices. Both applications rest on the fast (10 ns) and reversible transformation between the crystalline and amorphous phases induced by heating either via laser irradiation (DVD) or Joule effect (PCM). The two states of the memory can be discriminated thanks to the large difference in optical reflectivity and electronic conductivity of the two phases.

In this seminar, I will review the insights gained from atomistic simulations on the structural and functional properties of the prototypical  $Ge_2Sb_2Te_5$  and GeTe phase change compounds. Molecular dynamics simulations based on Density Functional Theory revealed a complex structure of the amorphous phase which displays a coexistence of tetrahedral and octahedral-like local geometries [1]. Calculations of the electronic properties of the crystalline and amorphous models provided a microscopic understanding of the origin of the electronic contrast between the two phases exploited in the devices [2]. Finally, the microscopic origin of the fast crystallization speed has been addressed by large scale simulations (tens of thousand atoms for tens of ns) based on an interatomic potential generated by fitting a DFT database with a Neural Network method [3]. Direct molecular dynamics simulations of the crystallization kinetics [3] revealed that the high crystal growth velocity is due to the persistence of a high atomic mobility in the liquid at high undercooling which is in turn the result of the fragility of the liquid and the appearance of dynamical heterogeneities.

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**#018 - Continuum modeling of heteroepitaxial growth: elastic relaxation, surface-energy minimization, misfit dislocations and intermixing.**

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Lattice-mismatched heteroepitaxial growth is nowadays a key step involved in the fabrication of a multitude of devices. However, full control over the different, sometimes competing phenomena taking place during deposition [1] has yet to be reached. Simulations can be precious in limiting the growth-parameter space to be sampled in actual experiments when searching for the desired system morphology.

In this work we present a continuum approach able to tackle heteroepitaxy while matching typical experimental sizes and time scales. Starting from a suitable free-energy functional describing both elastic and surface energy, evolution is described based on a surface-diffusion model including an external flux. A convenient and general description of surface-energy anisotropy (allowing us to simulate faceting also in the "strong anisotropy" regime) is introduced [2] and several illustrative applications to semiconductors are described, exploiting both Phase-Field and sharp-interface approaches. Successful comparison with experiments is demonstrated for qualitatively different systems.

We also discuss our attempt to simultaneously tackle elastic and plastic relaxation. In particular, we show how the stress field associated with an assigned distribution of misfit dislocations can be computed on the fly, its contribution to the surface chemical potential deeply influencing the growth mode.

It must be noted that for miscible systems, such as Ge/Si, the above set of phenomena is not yet sufficient to yield a realistic description of the growth process. At high growth temperatures, indeed, entropy of mixing can lead to significant surface exchanges between deposited and surface atoms. Tackling intermixing is possible, but it requires for a considerable extension of the formalism [3,4].



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### #019 - Ab initio electronic structure, optical, and magneto-optical properties of MnGaAs digital ferromagnetic heterostructures

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We report on a theoretical study of the electronic, optical, and magneto-optical properties of digital ferromagnetic heterostructures based on Mn  $\delta$ -doped GaAs. We consider different structures corresponding to Mn contents within the range 12%–50% and we study how the system changes as a function of the doping concentration. Our first-principles approach includes the spin-orbit interaction in a fully relativistic pseudopotential scheme and the local-field effect in the description of the optical absorption. We show that Mn  $\delta$ -doped GaAs shares many properties with the uniformly doped Ga  $1-x$  Mn  $x$  As system, i.e., half-metallicity, similar absorption spectra, and moderate Kerr rotation angles in the visible spectral region.

### #020 - Inhomogeneous electron gas in nanowire-based radial heterostructures.

Guido Goldoni - University of Modena and Reggio Emilia

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*Radial* heterostructures, based on the lateral overgrowth of free-standing nanowires constitute a flexible new class of multi-layered nanomaterials, where engineering of extended quantum states in the radial direction is possible, which are not strictly 1D or 2D. Similarly to traditional *planar* multilayers, but with the additional complexity of the polygonal symmetry inherited from the nanowire substrate, such core-shell nanowires may host *wrapped* heterojunctions or (multi-)quantum wells with remote doping, forming an electron gas which is naturally inhomogeneous, with coexisting coupled quasi-1D and quasi-2D channels.

Traditional methodologies for probing quantum states, such as transport in strong magnetic fields and inelastic light scattering, may be applied to radial heterostructures, but with additional complexities due to the peculiar symmetry. Furthermore, complex composition modulations over tens of nanometers, discrete symmetry of typical samples and self-consistent formation of the electron gas should be included in any computational model with predictive quality. In this talk, I will discuss recent theoretical predictions for the electron gas excitations in GaAs/AlGaAs radial heterostructures, the formation of magnetic states in the quantum Hall regime, and their spectroscopic signatures, in connection with recent intra- and inter-band spectroscopic investigations.

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### #021 - Local vs. macroscopic properties in semiconductors; the role of atomic hydrogen

Francesco Filippone - CNR - Istituto di Struttura della Materia

In GaAsN dilute alloys, small contents of the iso-electronic N impurity induce striking effects on the GaAs energy gap. This phenomenon has been explained in terms of a band anti-crossing interaction between electronic levels induced by the N impurity in the conduction band (CB) and GaAs levels at the CB bottom. On the other hand, there was a scarce knowledge

about the local properties of the N impurity, like the local electronic properties and chemical bonding, as well as on their relationships with the N effects on the GaAs band structure. In the present work, we will address such an issue by focusing on the role played by atomic hydrogen in the investigation of the N local properties.[1] Hydrogen binds indeed to impurities and modifies their local environment.[2] Here, we will discuss how this modification may be interpreted in terms of mutation of the impurity chemical environment by approaching this phenomenon on the side of theory.

Moreover, we will discuss as a parallel case, the effects of the introduction of atomic H in InGaN alloys. In these materials, indeed, a significant change of the host band structure is accompanied by the formation of multi-hydrogen complexes. [3]

In detail, we shall mainly present results from DFT calculations, with plain GGA, hybrid and GGA+U functionals (set up similar to ref. [4]), to be connected with relevant results from X-ray absorption and X-ray emission spectroscopies, as well as from photoluminescence spectroscopies.

The hydrogen complexes here proposed are analyzed both in their structural and electronic properties. A look at the most recent findings in the topic is given.

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#### #022 - Ab initio analysis of hyperfine structure in chalcogen-doped silicon and germanium nanowires: a route through a spin based quantum computer

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The localization of the donor electron wave function can be of key importance in various semiconductor application, since it determines the interactions between neighboring donors and influences the charge density close to the donor atom. These properties are important in light of applications like nuclear spin qubits [1] based on the hyperfine interaction between electron and nuclear spin [2]. In particular the delocalization is a critical feature when dealing with nanostructures, where the confinement induces a squeezing of the donor wave function.

In this contribution we employ ab initio density functional calculations with projector augmented-wave method (PAW) [3,4] to explore the hyperfine structure of S and Se substitutional defects in silicon and germanium nanowires. We show that, if the tetrahedral symmetry is preserved, the hyperfine contact term is only marginally dependent on the nanowire orientation, while it can undergo drastic changes if the symmetry is lost. In addition, we present a detailed analysis of the effect of compressive and tensile strain on the hyperfine parameters for Se doped Silicon nanowires, highlighting common features and differences among the three orientations considered. Based on our results, we demonstrate the [011] oriented nanowires as promising candidates for spin qubits applications, in particular if strain manipulation is considered.

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#### #023 - Kinetic Lattice Monte Carlo simulations and electronic transport of graphene with hydrogen

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The electronic structure of graphene can be greatly modified by hydrogen absorption, leading to modified electronic transport properties.

We simulate the dynamics of hydrogen adatoms absorbed on top of graphene, using the Kinetic Lattice Monte Carlo approach, which allows us to stochastically study large time and space scales. We model diffusion, as a thermally activated process, which needs to overcome an energy barrier given by the sum of a migration energy and a short-ranged hydrogen adatoms interaction energy, accounting for the stability of the local configuration. This interaction energy is made to depend only on the coordination of the adatoms, according to an Ising-like model, extending up to third nearest neighbors and is tested against Density Function Theory (DFT) results. Atomic and associative desorption of hydrogen adatoms are also considered and corresponding energy barriers are also estimated based on DFT computations, while atomic absorption occurs at a constant rate, fixed by an effective external atomic flux. The effect of different calibration choices are also shown.

Finally, the obtained structures are discussed and their electronic transport properties are investigated.

Computations are carried out for various temperatures and fluxes.

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**#024 - Transport processes in chaotic magnetic field configuration: the Quasi-Single-Helicity states in RFX-mod**

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Magnetic field lines embedded in a plasma confinement system are often characterized by a chaotic motion, that can lead to the degradation of the confinement properties of the system. However, even in case of chaotic domains, magnetic barriers can emerge and limit the field line motion itself.

Recently a fluid dynamical approach for the detection of these barriers has been developed [1, 2]. The method relies on the behavior of the Finite Time Lyapunov Exponent (FTLE) field, associated to the magnetic configuration. This FTLE field shows the presence of ridges, that can be recognized as Lagrangian Coherent Structures (LCSs) for the magnetic field, and act as barriers for the transport of magnetic field lines across them.

Here we provide the first application of this method to a real magnetic configuration [3]. We consider the magnetic field characterizing the emergence of self-organized quasi-helical states [4], predicted by magnetohydrodynamic (MHD) simulations [5] and observed in high current experiments in the reversed field pinch configurations.

We show that the LCSs we find actually limit the field lines motion and provide a chaos healing

effect, by influencing the transport properties of the system.

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**#025 - Neutron and gamma ray spectroscopy for diagnosing fast ions in burning plasmas**

*Marco Tardocchi (I) - IFP-CNR*

In thermonuclear fusion experiments devoted to study high power Deuterium (D) and Deuterium-Tritium (DT) plasmas the fuel ions are central for achieving high fusion powers. In the road towards the goal of a DT burning plasma one would like to achieve a Maxwellian thermal population of confined deuterons and tritons with high ion temperatures in the range 15 to 20 keV. Measurement of the D and T fuel ion energy distribution are important in order to assess the amount of thermal to suprathermal ion fraction, the latter created by the presence of external heating in the form of Ion Cyclotron Resonance Heating or Neutral Beam injection. At the same time, in today's fusion experiments investigation of fast ions is carried on and motivated by the need to understand and eventually control the instability associated to the shear Alfvén wave driven by suprathermal ions.

As the energy of the fast ions is increased towards the MeV range, such as that expected in next step fusion devices devoted to study DT burning plasmas, many of the techniques used today present principle and technical limitations which limit their applicability and nuclear diagnostics must be instead employed. Interesting candidates are represented by high resolution neutron (NES) and gamma ray emission spectroscopy (GRS), as demonstrated in recent experiments at the Joint European Torus (JET). In this talk the state of the art of NES and GRS instrumentation will be presented together with a review of the most recent results on JET plasmas.

A high resolution measurement of the neutron spectrum can provide insights on the fuel ion distributions. Through suitable modelling the bulk ion temperature and the high energy tail temperature can be extracted. Due to the enhanced fusion reactivity, NES measurements diagnose well a minority fraction of fuel fast ions, and in certain case, also the presence of the energetic fusion products (such as He3 or He4) via the so called "knock-on" secondary processes. GRS measurements with high energy resolution of fusion plasmas are recent and several nuclear reactions resulting in measurable levels of gamma ray emission have been observed in JET. The most common reactions occur between fast ions accelerated by ICRH and light plasma impurities, e.g. reactions involving fast H, D, <sup>3</sup>He and <sup>4</sup>He ions and Carbon or Beryllium impurities. Each reaction emits characteristic gamma rays with different energies; the intensities of the gamma peaks are related to the energy distribution of the fast ions, weighted by the underlying cross sections. GRS will be important on ITER for the diagnose of confined fusion alpha particles via the detection of 4.5 MeV gamma rays emitted from the reaction <sup>9</sup>Be(α, n)<sup>12</sup>C.

Finally, the status of the NES and GRS measurements planned for ITER will be reviewed.

### #026 - The coupling impedance as a tool for describing the self-consistent local and nonlocal effects induced by a relativistic driving beam in plasmas

Renato Fedele - Università di Napoli Federico II, Dipartimento di Fisica

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We describe the self-consistent interaction of a relativistic charged-particle beam with the surroundings while propagating through a plasma-based acceleration device. This is accomplished within the framework of the Vlasov-Maxwell system of equations for the system "plasma + beam". In full analogy with the conventional accelerators, here the interaction with the beam and the surrounding plasma is schematized in terms of the so-called "beam coupling impedance" (both longitudinal and transverse) which seems a very useful tool for the Nyquist-type stability analysis. Examples of specific physical situations are suitably illustrated.

### #027 - Turbulence in magnetized non-neutral plasmas

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Other Authors: Shi Chen (INFN Sezione di Milano and Institute of Fluid Physics, China Academy of Engineering Physics, Mianyang, Sichuan, China), Giancarlo Maero (INFN Sezione di Milano and Università degli Studi di Milano).

Magnetically confined electron plasmas evolve as essentially inviscid, incompressible two-dimensional (2D) fluids with a single sign of vorticity, allowing a quantitative study of shear flow instabilities, vortex formation and dynamics, turbulence and self-organization [1]. The dynamics of a pure electron plasma has been investigated both experimentally with the Penning-Malmberg trap ELTRAP [2] and numerically with two-dimensional (2D) particle-in-cell (PIC) simulations [3]. The analysis of the experimental and numerical data is based on the use of advanced techniques like wavelets and Proper Orthogonal Decomposition and on the determination of the statistical scaling properties of the electron density fluctuations [4, 5]. In particular, these studies highlight the role played by the initial conditions and by the density fluctuations on the early dynamics of the flow [6], leading eventually to the persistence of coherent structures and to the formation of vortex crystal-like states. Another factor of influence on both the dynamics and final state of the flow is the presence of a second species of charged particles. In particular, the contamination of the electron sample by micrometric-sized dust featuring an extremely large mass-to-charge ratio (complex plasma) is currently being investigated with 2D PIC simulations where the electron-dust system is described with a fluid-kinetic treatment. The effects of dust on the stability, insurgence of diocotron modes and fluid turbulence properties of the electron component are compared to the case of a pure electron plasma. Perspectives for the experimental investigation of the complex non-neutral plasmas are given.

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### #028 - Plasmonics effects in relativistic High Field regime: from electron acceleration to High Harmonics Generation

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Fine control of Electromagnetic Field coupling with structured metal surfaces is a vibrant research field (Plasmonics), with several interesting applications and a well developed theory. Plasmonics experiments are usually performed with low-intensity laser pulses. In this contribution we discuss the observation of plasmonics effects in ultra-high intensity laser-plasma interaction (peak intensity greater than  $10^{18}$  W/cm<sup>2</sup>). This regime, where relativistic, strongly non-linear effects are expected to take place, is essentially unexplored.

In a recent experiment performed at CEA-Saclay (France) we demonstrated for the first time electron acceleration by relativistic surface plasmons driven on a grating target at laser intensities greater than  $10^{19}$  W/cm<sup>2</sup> (fully relativistic). We observed a strong enhancement of both energy and flux of electron emission from grating targets compared to simple flat targets. Moreover, electrons were emitted within a narrow cone along the grating target surface. 3D Particle-In-Cell simulations performed with the open-source Particle-In-Cell code PICCANTE reproduce the experimental results with excellent agreement and provide useful insights to understand the physical processes at play.

In this contribution we discuss also the effect of the field enhancement associated with the excitation of a Surface Plasmon on High Harmonic Generation from gratings via particle-in-cell simulations performed with PICCANTE code.

The results we present may open the way for the extension of other plasmonics schemes into the ultra-high intensity regime, potentially with a broad range of interesting developments.

**#029 - Advanced active feedback schemes for MHD studies in hot magnetized plasmas**

Tommaso Bolzonella - Consorzio RFX

Other Authors: Matteo Baruzzo (Consorzio RFX), Paolo Bettini (Universita' di Padova e Consorzio RFX), Giuseppe Marchiori (Consorzio RFX), Leonardo Pigatto (Universita' di Padova e Consorzio RFX), Fabio Villone (Universita' di Cassino)

Magnetized plasmas represent a very good example of macroscopic complex systems where long and small range dynamics typical of neutral fluids are further complicated by electro-magnetic interactions. Increasing our understanding of laboratory based magnetized plasmas within the magneto-hydrodynamic (MHD) framework is important also to advance our knowledge on some basic phenomena of astrophysical plasmas such as ideal MHD, resistive reconnection and magnetic dynamo.

RFX-mod is a toroidal experimental facility operated by Consorzio RFX in Padova, capable of confining hot ( $T_e > 1\text{keV}$ ) hydrogen, deuterium or helium plasmas by the application of magnetic fields up to 0.6 T. The plasma is confined in toroidal geometry with major radius  $R=2\text{m}$  and minor radius  $a=0.46\text{m}$ . Thanks to its flexibility, RFX-mod can explore different magnetic configurations including the so called tokamak, Reversed Field Pinch, low- $q$  and ultra low- $q$ , each of which exhibits specific MHD stability properties. A peculiar feature of RFX-mod is the additional presence of a set of 192 active coils entirely covering the toroidal outer surface of the plasma [1]. These coils can be independently fed and are controlled by a fast (duty cycle of few ms) real time control software where different external "reactions" to plasma MHD activity can be implemented. This allows a unique flexibility in imposing different boundary conditions to MHD dynamics and in studying how to optimize the magnetic field properties in view of improving the MHD stability margins of the configuration confining the plasma [2,3].

Purpose of the present work is to present recent experimental results obtained in RFX-mod that significantly contribute to the wider effort of efficiently confine a fusion relevant plasma. In particular we will show detailed experiments where the intrinsic 3D nature of the stability problem is highlighted by properly manipulating the structure of the magnetic field produced by the 192 external coils [4]. The definition of the so-called "mode rigidity" will be critically reinterpreted for the case of the ideal kink instability developing in the presence of resistive passive and active magnetic boundaries. In the final discussion we will explain how these investigations not only allow a deeper understanding of the physics mechanisms underlying MHD stability in RFX-mod plasmas, but also constitute a subject where Consorzio RFX is providing an important support to the design and realization of new international magnetic fusion facilities such as JT-60SA in Japan and ITER in France.

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**#030 - Molecular spin in a quantum box**

Marco Affronte (I) - università di Modena e Reggio Emilia & CNR NANO

Other Authors: claudio bonizzoni, alberto ghirri

Molecular spins have demonstrated to be additional resources for encoding (quantum) bits [1]. This knowledge can now be exploited to fabricate quantum devices where functionalities of molecular spins are combined with other active nano-systems [2]. Here, we focus on the case in which molecular spin ensemble is in resonance with photons in a quantum box and eventually enter in a strong coupling regime, as described in the Tavis-Cummings model. To this end, I shall first illustrate our design and fabrication of microwave planar resonators operating as quantum box in a simple and cryogenic set up. X-band EPR spectra acquired at low temperatures allow us to extract the essential parameters of the low-lying energy levels of  $\text{Cr}_3$  and demonstrate that our set up is particularly suitable to study small crystals of molecular nanomagnets [3]. Secondly, I shall present the realization of YBCO microstrip resonators. The high quality factor (Q up to 30000) measured at high temperature (up to 70K) and in strong magnetic field (up to 7T) allow us to couple resonant photons (at 7.6GHz in our case) with several molecular spins including Cu and Co monomer or  $\text{ErPc}_2$  double decker. To prove that strong coupling regime can be achieved in these conditions, the evolution of frequency detuning and split of the resonant peak is reported as a function of temperature and magnetic field by using spin ensemble of DPPH organic radical [4].

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**#031 - Spotting X-ray light on molecular magnets: from bistability to magnetochirality**

Roberta Sessoli (I) - Università degli Studi di Firenze & INST, Dept. of Chemistry

Other Authors: Matteo Mannini

Molecules showing slow relaxation of the magnetisation, known as single molecule magnets (SMMs), have attracted significant interest as model systems in nanomagnetism, in particular for their rich quantum behaviour. Despite the difficulties hampering a significant increase of the operational temperatures these systems are nowadays investigated as new active units in molecular spintronics. The integration of SMMs in this type of devices requires that these molecules are either deposited on a substrate or inserted in nanogaps between electrodes. The intrinsic fragility of coordination compounds, combined with the elusive character of the molecular magnetic bistability, has limited the investigation to a few classes of molecules. We have obtained interesting results on a family of tetranuclear iron-based star-shaped clusters that can be either functionalized to be grafted on metallic surfaces or evaporated to be also embedded in vertical architectures behaving like spin-valves. Networks of gold nanoparticles bridged by  $\text{Fe}_4$  SMMs have also been obtained. The SMM behaviour and quantum features are retained also in these nanostructures.

The key tool for this type of research has been the use of synchrotron radiation, and in particular X-ray Magnetic Circular Dichroism, which has been employed at very low temperatures to evidence surface and element selective magnetic hysteresis in monolayers of molecules.

Hard X-rays have instead been employed to investigate molecular magnetic helices belonging to the class of compounds known or Single Chain Magnets (SCMs), i.e. one-dimensional structures showing magnetic hysteresis. Chiral magnetic structures have been recently the focus of intense research because they offer the possibility to store information in topological protected structures like skyrmions. Chirality and magnetism are also directly connected in the interaction between matter and electromagnetic radiation through the magneto-chiral dichroism and birefringence. A detailed synchrotron investigation at the 3d-metal K edge in two isostructural molecular helices comprising either isotropic Manganese(II) or anisotropic Cobalt(II) bridged by stable organic radicals has revealed a strong magneto-chiral dichroism associated with the non-collinear spin structure of the Co derivative, which is also the archetype of Single-Chain Magnets.

\*) The financial support of the European Research Council is acknowledged.

**#032 - Interface-driven effects in organic spintronic devices***Ilaria Bergenti (I) - ISMN CNR**Other Authors: V. Dediu (ISMN-CNR), A. Riminucci (ISMN-CNR), P. Graziosi (ISMN-CNR), M. Calbucci (ISMN-CNR), R. Cecchini (MDM-CNR), K. O'Shea (University of Glasgow)*

The driving force of inclusion of organic materials in spintronics is based on their longer spin lifetime of charge carrier with respect to conventional inorganic ones. Recently magnetoresistive devices have been obtained both in transport (long range) and tunneling (few nm) regimes [1,2]. Nevertheless these results need additional proofs than magnetoresistance to overcome the skepticism generated by the technological issues, like the poor definition of interfaces that is the main reason for the large variability of results in literature. Typical methods for measurement of spin transport in inorganic spintronic devices like measurements of spin precession of charges by Hanle effect do not succeed in having a clear response to this issue [3]. On the other hand, improvement of interface quality between organics and ferromagnets allowed to identify the primary role of interfacial hybridization in spin injection as well as allow to detect a series of effects able to give rise to possible new applications: between them bistability a non volatile memory effect [4].

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**#033 - The route towards interface-assisted molecular spintronics: from ferromagnetic metals to spin-textured materials***Mirko Cinchetti (I) - University of Kaiserslautern*

One very efficient route to tailor the spin properties of surfaces and interfaces, which was so far only applied to ferromagnetic metals, is the creation of customized hybrid interfaces between inorganic and organic materials. The interest in the spin properties of such systems was originally stimulated by the observation of magneto-resistive effects in spin-valve structures prepared with an organic-based spacer layer [1, 2]. Today, it is known that the performance of such organic spintronics devices is mostly determined by the spin-dependent properties of the hybrid interface formed between the organic molecules and the ferromagnetic electrodes: the so-called *spinterface* [3]. Crucially, the spin properties of a specific spinterface such as spin polarization, spin filtering, and coercive field can be in principle tuned by any external stimulus that will either modify the electronic structure of the organic molecules forming the spinterface, or change the strength of the interaction between the molecules and the ferromagnetic substrate. This concept was demonstrated, for example, for doping of the organic molecules with electron donors [4] and for chemical synthesis of tailored molecules [5, 6].

In this talk I will show that the extreme multi-functionality of organic molecules can be used to functionalize the spin properties of the more general class of spin-textured materials, opening new and exciting routes for controlling spin at the atomic scale [7]. In particular, I will present a rational design approach to customize the spin-texture of surface states of the prototypical topological insulator (TI)  $\text{Bi}_2\text{Se}_3$  [8]. For the rational design we use theoretical calculations to guide the choice and chemical synthesis of appropriate molecules that customize the spin-texture of  $\text{Bi}_2\text{Se}_3$ . The theoretical predictions are then verified in angular-resolved photoemission experiments. We show that by tuning the strength of molecule-TI interaction, the surface of the TI can be passivated, the Dirac point can energetically be shifted at will, and Rashba-split quantum-well interface states can be created. These tailored interface properties lay a solid foundation for interface-assisted molecular spintronics in spin-textured materials.

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[8] S. Jakobs, ..., O. Monti, M. Aeschlimann, R. J. Cava, M. Ruben, S. Mathias, S. Sanvito, and M. Cinchetti, *under review* (2015).**#034 - Looking Inside the Paramagnetism of Perchlorinated Trityl Radical/Metal Spinterface through Spectroscopy***Maddalena Pedio - CNR IOM/TASC**Other Authors: Veronica Mugnaini, (Materials Science of Barcelona (ICMAB-CSIC)/CIBER-BBN, Cerdanyola, Spain) Albano Cossaro (CNR-IOM, TASC Area Science Park, Basovizza, Trieste, Italy), Cinzia Cepek (CNR-IOM, TASC Area Science Park, Basovizza, Trieste, Italy), Mathieu Gonidec (Materials Science of Barcelona (ICMAB-CSIC)/CIBER-BBN, Cerdanyola, Spain), Isaac Alcon (Materials Science of Barcelona (ICMAB-CSIC)/CIBER-BBN, Cerdanyola, Spain), Ruslan Ovsyannikov (Helmholtz Zentrum Berlin für Materialien und Energie, BESSY II, Berlin, Germany), Antje Vollmer (Helmholtz Zentrum Berlin für Materialien und Energie, BESSY II, Berlin, Germany), Arrigo Calzolari (CNR-NANO Istituto Nanoscienze S3 National Center, Modena, Italy), Jaume Veciana (Materials Science of Barcelona (ICMAB-CSIC)/CIBER-BBN, Cerdanyola, Spain), Manvendra Kumar (CNR-IOM, TASC Area Science Park, Basovizza, Trieste, Italy),*



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Persistent and stable organic molecules with an open-shell electronic configuration have long been known and extensively studied mainly in solution. Only recent is instead the study of organic radicals as laterally self-assembled monolayers immobilized on substrates towards their application in devices, e.g. in organic spintronics [1,2]. To exploit this latter field of applied research, the knowledge of the electronic properties of the organic side of the organic radical/metal interface is of primary importance. We report on a spectroscopic multitechnique approach (photoemission spectroscopy, inverse photoemission spectroscopy and near-edge X-ray absorption fine structure spectroscopy) to study the metal/radical spinterface formed by a perchlorinated trityl radical derivative and either gold or silver. The spectroscopic fingerprint of their paramagnetic properties could be determined by comparison with their diamagnetic precursor and by DFT calculations. Thanks to the presented approach, we could gain unprecedented insight into the radical-metal interaction and how this latter perturbs the spin polarization and consequently the magnetoelectronic properties of the radical adlayer. Knowledge of the factors influencing the spinterface is an essential tool toward the tailoring of the properties of spin-based electronic devices. References [1] J. Liu, H. Isshiki, K. Katoh, T. Morita, B- K. Breedlove, M. Yamashita, T. Komeda, *J. Am. Chem. Soc.* 2013, 135, 651–658; S. Sanvito, *Chem. Soc. Rev.* 40 (2011) 3336-3355. [2] Veronica Mugnaini, Arrigo Calzolari, Ruslan Ovsyannikov, Antje Vollmer, Mathieu Gonidec, Isaac Alcon,† Jaume Veciana, Maddalena Pedio *J. Phys. Chem. Lett.*, 6 (2015) 2101–2106

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**#035 - Soft electronic matter in underdoped cuprates**

Sergio Caprara (I) - Sapienza Università di Roma - Dipartimento di Fisica

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Empirical evidence in heavy-fermion materials, pnictides, and other systems suggests that unconventional superconductivity appears associated to some form of real-space electronic order. For the high- $T_c$  superconducting cuprates, despite several proposals, the emergence of order in the region of the phase diagram between the commensurate antiferromagnetic state and the superconducting state is not well understood. We show that in this regime the doped holes assemble in “electronic polymers”. Within a Monte Carlo study we find that in clean systems by lowering the temperature the polymer melt condenses first in a smectic state and then in a Wigner crystal both with the addition of inversion symmetry breaking. Disorder blurs the positional order leaving a robust inversion symmetry breaking and a nematic order, accompanied by vector chiral spin order and with the persistence of a thermodynamic transition. Such electronic phases, whose properties are reminiscent of soft-matter systems, produce charge and spin responses in good agreement with experiments.

**#036 - Ultrafast snapshots of the fundamental interactions in cuprates**

Claudio Giannetti (I) - Università Cattolica del Sacro Cuore

Time-resolved techniques have opened a new window on the ultrafast microscopic processes in high-temperature superconductors and strongly-correlated materials. The ultimate goal of this real-time approach is the clarification of the pairing mechanism in high-temperature superconductors [1], as well as the development of new tools to manipulate the fundamental interactions by means of ultrashort light pulses.

Here we present some recent time-domain results on superconducting copper oxides. By simultaneously pushing the time resolution and frequency range of transient reflectivity measurements, we directly observed the  $\sim 16$  fs build-up of the effective electron–boson interaction [2]. This extremely fast timescale strongly points to magnetic excitations as the fundamental mediators of the electronic processes in cuprates.

Furthermore, we investigated the dynamics of the high-energy ( $\sim 2$  eV) charge-transfer process in the single-layer  $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+6}$  cuprate. We demonstrated that there is a critical doping,  $p_{cr}=0.16$ , which marks a transition in the nature of the Cu-O wavefunctions, that evolve with doping from localized, as in a Mott insulator, to delocalized, as in a conventional metal. Since this phenomenon is observed at room temperature, we conclude that there exists a common correlated state, characterized by the freezing of the local  $\text{O}-2p \rightarrow \text{Cu}-3d$  charge fluctuations, which is precursor to the symmetry-broken instabilities, such as charge-ordering, that develop at low doping and temperature.

[1] S. Dal Conte et al. *Snapshots of the retarded interaction of charge carriers with ultrafast fluctuations in cuprates*. Nat. Phys. 11, 421 (2015).

[2] S. Dal Conte et al. *Disentangling the electronic and phononic glue in a high- $T_c$  superconductor*. Science 335, 1600–1603 (2012).

**#037 - Charge order in Cuprates from strongly correlated Fermi Liquid to low doped anti-ferromagnet**

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Charge order in Cuprates from strongly correlated Fermi Liquid to low doped anti-ferromagnet

Carlo Di Castro

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Collaborators: Capati, Caprara, Grilli, Lorenzana, Seibold.

I will outline how heterogeneous states in the entire pseudogap region form a bridge between highly-doped Fermi-Liquid and low-doped anti-ferromagnet. Quasi-critical fluctuations of various nature mark the evolution of the heterogeneous state with specific signatures in the spectroscopic properties (Arpes, Raman).

Charge order, elusive until 2012, is now ubiquitously observed in cuprates. Theoretically, an incommensurate charge density wave instability of the strongly correlated Fermi-Liquid is marked by a critical line, which ends in a hidden quantum critical point at  $T=0$  and closely tracks the pseudogap temperature  $T^*$  as the onset of heterogeneity.

Crossover from charge to spin promoted order by lowering the doping is well accounted for by a phenomenological Fermion-Boson model for fitting Arpes and Raman experiments.

At very low doping, the doped charges aggregate in polarized segments precursors of stripes. In clean systems by lowering the temperature these "electronic polymers" condense in a smectic state and then in a Wigner crystal phases both with inversion symmetry breaking. Disorder smears the positional order and leaves a polarized nematic phase with a vector chiral spin order, well reproducing neutron scattering experiments.

G. Seibold et al, PRB 87, 035138 (2013); M. Capati et al, Nature Comm. July (2015); S. Caprara et al, Phys. Rev. B 84, 054508 (2011). G. Mazza et al, Phs. Rev. B 87, 014511 (2013).

### #038 - Magnetic excitations and phonons simultaneously studied by resonant inelastic x-ray scattering in optimally doped $\text{Bi}_{1.5}\text{Pb}_{0.55}\text{Sr}_{1.6}\text{La}_{0.4}\text{CuO}_6$

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Understanding the unusual physical properties of high temperature superconductors, and superconductivity mechanisms therein, remains one of the main challenges in condensed matter physics. Recently, resonant inelastic x-ray scattering (RIXS) at the  $\text{Cu } L_3$  edge, which provides a direct access to spin-flip excitations, has become a powerful tool, complementary to neutron inelastic scattering, for the determination of the magnetic-excitation dispersion in cuprates. Magnetic excitations have thus been observed from undoped antiferromagnetic insulators to overdoped superconductors for hole- and electron-doped compounds, demonstrating the robustness of magnetic fluctuation across the superconducting phase diagram. Moreover,  $\text{Cu } L_3$  resonant soft x-ray scattering has decisively contributed to reveal a charge order that competes with superconductivity: initially seen in  $(\text{Y,Nd})\text{Ba}_2\text{Cu}_3\text{O}_{6+x}$  charge order is now considered ubiquitous in cuprate superconductors. The interest of RIXS can be further extended, because in correlated solids almost all types of excitation (charge, spin, orbital and lattice) can be probed by RIXS. As some (if not all) of these excitations are commonly believed to play a significant role in the superconductivity of cuprates, the investigation on whether and how they mutually interact and mix can be of highest importance.

Here we study, by high resolution  $\text{Cu } L_3$  RIXS, the magnetic excitations in the optimally doped high- $T_c$  superconductor  $\text{Bi}_{1.5}\text{Pb}_{0.55}\text{Sr}_{1.6}\text{La}_{0.4}\text{CuO}_{6+d}$  (OP-Bi2201,  $T_c \approx 34$  K), below and above the pseudogap opening temperature. At both temperatures the broad spectral distribution disperses along the  $(1,0)$  direction up to  $\sim 350$  meV at zone boundary, similarly to other hole-doped cuprates. However, above  $\sim 0.22$  reciprocal lattice units, we observe a concurrent intensity decrease for magnetic excitations and quasi-elastic signals with weak temperature dependence. This anomaly seems to indicate a coupling between magnetic, lattice and charge modes in this compound. We also compare the magnetic excitation spectra near the anti-nodal zone boundary in the single layer OP-Bi2201 and in the bi-layer optimally doped  $\text{Bi}_{1.5}\text{Pb}_{0.6}\text{Sr}_{1.54}\text{CaCu}_2\text{O}_{8+d}$  (OP-Bi2212,  $T_c \approx 96$  K). The strong similarities in the paramagnon dispersion and in their energy at zone boundary indicate that the strength of the super-exchange interaction and the short-range magnetic correlation cannot be directly related to  $T_c$ , not even within the same family of cuprates.

### #039 - Optical and transport properties of epitaxial $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ thin films

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Electrical transport measurements and transient optical pump-probe experiments have been performed on epitaxial films of the electron doped  $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$  compound for studying the non-equilibrium carrier dynamics in this material. In particular, the value of the quasiparticle relaxation time has been estimated in order to investigate the possible use of this compound as base material for superconducting optical detectors. Samples have been grown on (001)-oriented  $\text{SrTiO}_3$  substrates by dc sputtering in a mixed atmosphere of both Ar and  $\text{O}_2$ . X-ray diffraction analysis and Scanning Electron Microscope equipped with a wavelength dispersive spectroscopy detector have been used to characterize the structure and the morphology and composition of the thin films. Time-solved femtosecond pump-and-probe spectroscopy has been also carried out on our samples in the temperature range 4.2K-300 K. The data demonstrate a clear correlation between electrical and optical features.

**#040 - Multiband BCS superconductivity at low density**

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The interplay between electronic density and critical properties assumes a fundamental role in the understanding of many recently discovered superconductors. In turn, geometry, dimensionality, quantum confinement, multiband effects, are all factors that contribute to the modulation of the critical temperature  $T_c$  as a function of carrier density. These dependences are particularly relevant for low-density systems, characterized by a chemical potential that approaches the electronic band edge; such materials include SrTiO<sub>3</sub>, thin superconducting films, the LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface. In this work, we explore the consequences of band-edge effects in the framework of BCS theory, developing a formalism for different dimensionality, and multiband configurations. The model is subsequently applied to superconducting thin films, within the context of shape resonances and shell effects; we show that the inclusion of low density effects ensures the continuity of  $T_c$  curves, that are significantly modified as a function of density and confinement length. Furthermore, the simultaneous characteristics of multiple bands and low density are investigated for the LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface, allowing for a comparison of interface superconductivity with respect to bulk SrTiO<sub>3</sub>.

**#041 - Local lattice displacements and superconductivity in BiS<sub>2</sub>-based layered materials**

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The recent discovery of superconductivity in RE(O/F)BiS<sub>2</sub> (RE = rare earth) has triggered theoretical and experimental efforts to understand the pairing mechanism. These materials show a layered structure with BiS<sub>2</sub> layers, which becomes superconducting after electron doping, alternated with rare-earth oxide layers which act as a charge reservoir. These properties are shared by unconventional superconductors like the cuprates and the iron based family. The analogy with these materials is enriched by the multiband nature of the Fermi surface, the indication of nesting and the coexistence of superconductivity and magnetism which are peculiar characteristics of iron based superconductors. Despite the relatively low  $T_c$  (maximum at 10.6 K) the debate between conventional and non-conventional pairing is still unsettled. A peculiar feature of the superconducting state is the high sensitivity to external pressure, chemical pressure and high pressure sample synthesis. This is a clear indication of a strong interplay between structural distortions and the transport and electronic properties in this class of materials. We have used X-ray absorption spectroscopy to study the effects of doping in the local structure and the valence electronic states in CeO<sub>1-x</sub>F<sub>x</sub>BiS<sub>2</sub>. We find that Bi-S local correlations evolve systematically with fluorine substitution bringing the system to a decoupling between the BiS<sub>2</sub> and CeO layer, hence coexistence of superconductivity and ferromagnetism [1,2]. Results will be discussed in the frame of an interplay between local structural deformations and electronic properties in CeO<sub>1-x</sub>F<sub>x</sub>BiS<sub>2</sub>. In addition, we have also investigated the effect of chemical pressure, which is known to dramatically affect superconductivity, by changing mean rare earth size. In particular the local effect of substitution of the rare-earth with Ce, Nd, Sm encompassing a wide range of ionic radius will be discussed [3].

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[2] E. Paris, B. Joseph, A. Iadecola, T. Sugimoto, L. Olivi, S. Demura, Y. Mizuguchi, Y. Takano, T. Mizokawa & N. L. Saini, J. Phys. Condens. Matter 26, 435701 (2014).

[3] Y. Mizuguchi, E. Paris, T. Sugimoto, A. Iadecola, J. Kajitani, O. Miura, T. Mizokawa, N. L. Saini, to be published (2015).

**#042 - The Hubbard model beyond the two-pole approximation: a Composite Operator Method study**

*Adolfo Avella - Università degli Studi di Salerno*

Within the framework of the Composite Operator Method, a three-pole solution for the two-dimensional Hubbard model is presented and analyzed in detail. In addition to the two Hubbard operators, the operatorial basis comprises a third operator describing electronic transitions dressed by nearest-neighbor spin fluctuations. These latter, compared to charge and pair fluctuations, are assumed to be preeminent in the region of model-parameter space – small doping, low temperature and large on-site Coulomb repulsion – where one expects strong electronic correlations to dominate the physics of the system. This assumption and the consequent choice for the basic field, as well as the whole analytical approximation framework, have been validated through a comprehensive comparison with data for local and single-particle properties obtained by different numerical methods on varying all model parameters. The results systematically agree, both quantitatively and qualitatively, up to coincide in many cases. Many relevant features of the model, reflected by the numerical data, are exactly caught by the proposed solution and, in particular, the crossover between weak and intermediate-strong correlations as well as the shape of the occupied portion of the

dispersion. A comprehensive comparison with other n-pole solutions is also reported in order to explore and possibly understand the reasons of such good performance.

**#043 - Optical feedback interferometry in THz quantum cascade lasers: Imaging of free carriers and all-optical metamaterials**

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We will review our recent results on a novel detectorless contact-free imaging method based on the use of THz quantum cascade lasers operating under optical feedback (self-mixing) to monitor the dielectric response and the free electron plasma photo-generated in a semiconductor surface, will be reviewed. This demonstration has paved the way to the use of periodic patterns of photo-excited carriers on a semiconductor surface to modify the effective permittivity and create all-optical quasi-metallic metamaterials. Intriguingly, one can artificially tailor the meta-material birefringence to modulate with unprecedented degrees of freedom both the amplitude and phase of a laser subject to optical feedback from such a reconfigurable anisotropic reflector.

**#044 - Photo-generated THz plasmonic antennas and metamaterials**

*Jaime Gomez Rivas (I) - FOM Institute AMOLF*

*Other Authors: George Georgiou, Arkabrata Bhattacharya*

Optical illumination of semiconductors leads to photoinduced doping. When the illumination is local and intense, the semiconductor transitions from a dielectric to a metallic behavior at THz frequencies only at the illuminated area. We have used this concept to demonstrate experimentally the photo-excitation of THz localized surface plasmon polaritons (LSPPs) in flat semiconductor layers [1]. This demonstration is realized by a patterned optical excitation of free charge carriers in thin films of GaAs using a spatial light modulator, which enables full spatial and temporal control of plasmonic resonances without the need of physically structuring the sample. This approach is also used to excite capacitively and inductively coupled LSPPs in loaded plasmonic antennas [2]. We also propose the spatially structured photoinduced doping of semiconductors to dynamically generate plasmonic waveguides and circuits [3]. Structured illumination also enables active beaming of THz radiation with planar structures [4].

[1] G. Georgiou, H.K. Tyagi, P. Mulder, G. Bauhuis, J. Schermer and J. Gómez Rivas, Photo-generated THz antennas, *Sci. Rep.* 4, 3584 1-5 (2014).

[2] G. Georgiou, C. Tserkezis, M.C. Schaafsma, J. Aizpurua and J. Gómez Rivas, Active loaded plasmonic antennas at terahertz frequencies : Optical control of their capacitive-inductive coupling, *Phys. Rev. B* 91, 125443 1-7 (2015)

[3] H.K. Tyagi and J. Gómez Rivas, Photo-generated THz plasmonic waveguides, *J. Opt.* 16, 094011 1-7 (2014).

[4] T.P. Steinbusch, H.K. Tyagi, M.C. Schaafsma, G. Georgiou and J. Gómez Rivas, Active terahertz beam steering by photo-generated graded index gratings in thin semiconductor films, *Opt. Express* 22, 26559-26571 (2014).

**#045 - Optical control of comb emission in mid infrared quantum cascade lasers**

*Francesco Cappelli - CNR-INO*

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Optical feedback and injection locking are two well established techniques allowing for the control of mid infrared quantum cascade lasers (QCLs) emission. The first one, with the laser mounted in an external cavity configuration [1], enables wide tunability of the source. On the other hand, the second one, implemented using a metrological-grade radiation as master [2], enables the transfer of the phase stability of the master oscillator to the QCL radiation.

Recently, comb operation in QCLs has been demonstrated [3]. Although a phase relation between the modes has been demonstrated, the comb emission has to be stabilized to be used for high-resolution spectroscopy applications. Optical techniques seem to be good candidates to this task. This aspect will be discussed in detail.

[1] A. Hugi, R. Maulini and J. Faist, "External cavity quantum cascade laser," *Semicond. Sci. Technol.* 25, 083001 (2010).

[2] S. Borri, I. Galli, F. Cappelli, A. Bismuto, S. Bartalini, P. Cancio, G. Giusfredi, D. Mazzotti, J. Faist, and P. De Natale, "Direct link of a mid-infrared QCL to a frequency comb by optical injection," *Opt. Lett.* 37, 1011-1013 (2012).

[3] A. Hugi, G. Villares, S. Blaser, H. C. Liu, and J. Faist, "Mid-infrared frequency comb based on a quantum cascade laser," *Nature* 492, 229-233 (2012).

**#046 - First-principles nonlocal homogenization theory for metamaterials**

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We discuss a simple first-principles homogenization theory for describing, in the long-wavelength limit, the effective bianisotropic response of a periodic metamaterial composite without intrinsic chiral and magnetic inclusions. Specifically, by resorting to a suitable multiscale technique, we show that medium effective permittivity tensor and the first and second order tensors describing spatial dispersion can be evaluated by averaging suitable spatially rapidly-varying fields each satisfying electrostatic-like equations within the metamaterial unit cell. As a leading example admitting full analytical description, we consider a simple multilayered periodic structure characterized by one-dimensional geometric chirality, i.e. its mirror image can not be superposed onto it by using translations without resorting to rotations. We show that the considered one-dimensional metamaterials are characterized by a bianisotropic response and support strong optical activity.

**#047 - Photo-generated THz plasmonic antennas and metamaterials**

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Optical illumination of semiconductors leads to photoinduced doping. When the illumination is local and intense, the semiconductor transitions from a dielectric to a metallic behavior at THz frequencies only at the illuminated area. We have used this concept to demonstrate experimentally the photo-excitation of THz localized surface plasmon polaritons (LSPPs) in flat semiconductor layers [1]. This demonstration is realized by a patterned optical excitation of free charge carriers in thin films of GaAs using a spatial light modulator, which enables full spatial and temporal control of plasmonic resonances without the need of physically structuring the sample. This approach is also used to excite capacitively and inductively coupled LSPPs in loaded plasmonic antennas [2]. We also propose the spatially structured photoinduced doping of semiconductors to dynamically generate plasmonic waveguides and circuits [3]. Structured illumination also enables active beaming of THz radiation with planar structures [4].

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[3] H.K. Tyagi and J. Gómez Rivas, Photo-generated THz plasmonic waveguides, *J. Opt.* 16, 094011 1-7 (2014).

[4] T.P. Steinbusch, H.K. Tyagi, M.C. Schaafsma, G. Georgiou and J. Gómez Rivas, Active terahertz beam steering by photo-generated graded index gratings in thin semiconductor films, *Opt. Express* 22, 26559-26571 (2014).

**#048 - Self-assembled Nanoparticles - Characterization and Application**

*Michael Gradzielski (I) - Technische Universität Berlin*

A rather flexible way to obtain functional, soft nanoparticles of various size and shape is via ionic assembly, for instance by employing charged (co)polymers and oppositely charged surfactants. Depending on the detailed molecular architecture of the polymers and the surfactants and their mixing ratio quite differently structured assemblies can be formed, where the local structure is typically dominated by the smaller surfactant molecules, while the overall structure and the stability depend strongly on the polymer.

By tuning the composition one then is able to obtain anything from densely arranged spherical micelles glue together by oppositely charged polyelectrolyte, over more extended rod-like structures up to rather loose complexes. Particularly interesting are in that respect biocompatible polymers such as chitosan or modified cellulose in combination with mild surfactants, such as alkylethoxy carboxylates or phospholipids. The formed complexes have mainly been characterized structurally by means of light and neutron scattering which yields a structural phase diagram. Depending on composition and pH one then has the option to vary the structures in a systematic way and also to control the flow properties over an extended range.

Finally we also give some examples how such systems may be employed for purposes of sequestration of organic compounds or metal ions. Accordingly such systems are promising candidates for developing nanostructured systems that are based biologically benign compounds and useful for a variety of applications.

**#049 - TiO<sub>2</sub> AND C BASED PHOTOCATALYTIC NANOMATERIALS FOR WATER PURIFICATION**

*Vittorio Privitera (I) - CNR-IMM*

The focus of the presentation is on the application of nanotechnology to water treatment [1, 2]. Worldwide 1.2 billion people suffer inadequate access to clean water. Nanotechnology is expected to improve the water purification with lower cost and energy. These were the major motivations for undertaking the initiative of the EU project WATER [www.water.imm.cnr.it](http://www.water.imm.cnr.it), coordinated by CNR-IMM, that aims to develop novel applications attracting industrial and service assets. The mineralization of organic compounds and the antibacterial efficiency of several nanomaterials and nanocomposites are reviewed, along with an evaluation of the nanotoxicology aspects related to the use of nanomaterials in the environment. Some examples are shown about TiO<sub>2</sub> nanoparticles, nanowires, nanotubes combined with metals, C or sensitizing molecules to increase the photocatalytic efficiency and modulate the range of light absorption [3-6]. Nanotech filtration up-scalable to industrial production might determine an impact on the economy and society through technology innovation. 1. Hu A. and Ablett A.; Nanotechnology for Water Treatment and Purification; Lecture Notes in Nanoscale Science and Technology 22; Springer 2014. 2. Savage N. et al.; Journal of Nanoparticle Research; 7, 331-342, 2005 Li Q. et al., Water Research; 42, 4591-4602, 2008. 3. G. Impellizzeri, V. Scuderi, L. Romano, P. Sberna, E. Arcadipane, R. Sanz, F. Simone, and V. Privitera. "Fe ion-implanted TiO<sub>2</sub> thin film for efficient visible-light photocatalysis", Journal of Applied Physics, Vol. 116, pp. 173507, 2014. 4. V. Scuderi, G. Impellizzeri, L. Romano, M. Scuderi, G. Nicotra, K. Bergum, A. Irrera, B. G. Svensson and V. Privitera. "TiO<sub>2</sub>-coated nanostructures for dye photo-degradation in water", Nanoscale Research Letters, Vol. 9, pp. 458, 2014. 5. R. Sanz González, L. Romano, M. Zimbone, M. A. Buccheri, V. Scuderi, G. Impellizzeri, M. Scuderi, G. Nicotra, J. Jensen and V. Privitera. "UV-black rutile TiO<sub>2</sub>: An antireflective photocatalytic nanostructure", Journal of Applied Physics, Vol. 117, pp. 074903, 2015. 6. V. Scuderi, G. Impellizzeri, L. Romano, M. Scuderi, M. V. Brundo, K. Bergum, M. Zimbone, R. Sanz González, M. A. Buccheri, F. Simone, G. Nicotra, B. G. Svensson, M. G. Grimaldi and V. Privitera. "An enhanced photocatalytic response of nanometric TiO<sub>2</sub> wrapping of Au nanoparticles for eco-friendly water applications", Nanoscale, Vol. 6, pp. 11189, 2014.

**#050 - Ion irradiation of frozen gases and astrophysical applications**

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Infrared observations allowed the detection of molecules in the solid phase as icy mantles on dust grains along the line of sight of quiescent molecular clouds and star forming regions. About 10 molecular species have been firmly identified in icy grain mantles and it is largely believed that many others, also complex species cannot be detected because of instrumental detection limits. Some of the observed species (such as CO) freeze out from the gas phase on the cold surface (4-100 K) of the dust grains, while others (such as H<sub>2</sub>O and CH<sub>3</sub>OH) are formed on grains after surface reactions. Other molecules (such as CO<sub>2</sub>, OCS) are not expected to freeze out from the gas phase and grain surface models do not account for their observed abundance. It has been suggested that these molecules, along with other more complex species, are products of the interaction between icy mantles and low-energy cosmic rays and UV photons. If the temperature increases, all these species are released to the gas phase after desorption of icy mantles and can be detected by radio astronomical techniques. Most of our knowledge on the physical and chemical properties of ices in star forming regions is based on the comparison between observations and laboratory experiments. In this work we report on some recent results obtained by irradiating frozen gases at low temperature (10-100 K) with energetic ions (keV-MeV, simulating



cosmic ions). Energetic ions passing through molecular solids release their energy to the target along the ion track. As a consequence chemical bonds are broken, rearranging the molecular and crystalline structure of the original sample. We used infrared and Raman spectroscopy to characterize the effects of irradiation. By means of infrared spectroscopy it is possible to identify molecular groups and specific molecules, while Raman spectroscopy gives further information about the structural properties of the samples and it is often used to study the effect of ion induced damage in carbonaceous solids. Some specific results obtained after ion bombardment of frozen CO, N<sub>2</sub>, CH<sub>3</sub>OH and their mixtures will be presented in light to their relevance to the astrochemical evolution of ices in star forming regions.

#### **#051 - Modification of graphene oxide and graphene oxide-TiO<sub>2</sub> solutions by pulsed laser irradiation for dye degradation**

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Carbon nanostructures have been already used as high-capacity and selective sorbents for organic solutes in aqueous solutions. In particular, graphene oxide (GO) and reduced graphene oxide (RGO) have been used as scaffold materials for photocatalytic nanoparticles showing higher binding capacity for different water contaminants than free nanoparticles. Furthermore, GO has shown photocatalytic properties and the ability of enhancing the activity of known photocatalyst as TiO<sub>2</sub>. This work reports the preparation of RGO by pulsed laser irradiation starting from commercial GO prepared by the modified Hummers method, in order to investigate any modifications of the photocatalytic properties after the reduction. Pulsed laser with visible wavelength (532 nm) is suitable to finely tune the degree of reduction and tailor both the hydrophilicity and the spectroscopic features of the final GO suspension. In addition, in this work pulsed laser irradiation is also used for producing mixed solution of GO and RGO with P25 titania. The produced materials are characterized by scanning electron microscopy (SEM), infrared, Raman and x-ray spectroscopy (XPS). The photocatalytic activity is investigated by studying the decolorization of methylene blue solution under UVA-visible and visible irradiation. Furthermore, the absorption of methylene blue and its aggregation on graphene layers is a direct measure of GO reduction and of its layer properties. The role of P25 titania in enhancing GO reduction under laser irradiation is suggested by XPS analysis and it will be investigated in more detail.

#### **#052 - Efficient photocatalysis by polymeric nanocomposites for water purification**

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In this work, we present TiO<sub>2</sub> based polymeric nanocomposites, combined with electron scavengers or sensitizers, as valid tools for water purification. Such nanocomposites have high photocatalytic and antibacterial activity; they were synthesized using poly (methyl methacrylate) as polymer matrix. These PMMA based materials are stable, harmless and cheap and they overcome many of the current issues that prevent the real application of the nanomaterials for water treatments, such as their dispersion in water and the consequent related toxicology aspects. We combined titanium dioxide with carbon nanotubes, as acceptor systems of electrons, and obtained a significantly higher photocatalytic efficiency under UV light for the activation of the degradation processes, compared to the efficiency of the systems with TiO<sub>2</sub> only. Furthermore, we synthesized operative materials even under visible light thanks to the functionalization of TiO<sub>2</sub> surface with sensitizers, such as porphyrins. This aspect is crucial for the application of TiO<sub>2</sub> as photocatalyst in the visible range, transferable to the industrial scale. We realized these polymeric nanocomposites by sonication and solution casting method. We evaluated their photocatalytic activity by degradation of dyes in an aqueous medium and we tested the antibacterial activity through CFU count using *Escherichia coli* as a model organism.

#### **#053 - Electron energy-loss spectra of graphene oxide for the determination of oxygen functionalities**

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Graphene based materials for large-scale production can be obtained starting from graphene oxide (GO) by means of suitable treatments, like thermal processes, chemical treatments or UV irradiation, in order to reduce the number of oxygen functional groups.

The presence of C-O bonds opens an electron energy gap that can be modulated between the insulating and the conductive behavior. Furthermore, the polar oxygen functional groups of GO render it strongly hydrophilic. Therefore, GO is highly dispersible in many solvents and it can be easily deposited by spraying, drop-casting or spin-coating for use in cheap technological applications. In addition, using well-known chemistry strategies, the oxygen functionalities can be utilized as sites for easy chemical modification

or functionalization of GO. All these aspects suggest the importance of the study and the individuation of the different oxygen functionalities of GO.

The composition and the structure of GO and reduced GO depend on the synthesis and reduction methodologies. In this work, GO was prepared by a modified Hummers method and reduced by pulsed laser irradiation using visible wavelength (532 nm). Transmission electron microscopy analyses were performed and dual electron energy-loss spectra were acquired in different regions of GO and reduced GO flakes. Experimental results show a series of characteristic peaks related to C and O K-edge shells. Density functional theory calculations of the high-loss region of the electron energy loss spectra at atomic level enable a reliable correlation between the observed experimental peaks and the presence of different oxygen functional groups (C-O-C, C-OH, O in vacancies) on the graphene surface.

#### **#054 - MW-Assisted synthesis of Ag nanoparticles using rosemary essential oil and their use to prepare silver-hydrogel nanocomposites**

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The synthesis and characterization of acrylamide based hydrogel loaded with silver nanoparticles by a two step methodology is shown in this work. First, silver nanoparticles (AgNPs) were synthesized using rosemary essential oil (EO) as renewable reducing agent in a green and fast microwave (MW) assisted process. Then, the in-situ free radical polymerization reaction of well-dispersed crosslinked acrylamide-based composite hydrogel containing the AgNPs was performed. This methodology is aimed by an innovative approach using a coaxial dipole antenna to apply the electromagnetic energy inside the aqueous medium in both: i) rosemary EO extraction by hydrodistillation and ii) silver nanoparticles synthesis at atmospheric pressure.

Nanoparticles formation was followed by UV-vis spectroscopy and SEM imaging. Silver nanoparticles with a tunable particle size (from 7 to 18 nm) were obtained. The polymeric nanocomposites, obtained by free radical polymerization process, were highly random materials built up by a main acrylamide backbone unit and partially crosslinked with methylene bis acrylamide (MBA). The nanocomposites properties were investigated by studying the swelling, rheological and thermogravimetric behaviour. Swelling capacity, viscoelastic properties and thermal stability were dependent on the dispersed AgNPs concentration into the polymeric network. These nanocomposites, which involve the use of green synthesis, are economically convenient and easily manipulated materials that can be used as carrier to apply the silver nanoparticles properties in very different applications.

**#055 - Infrared-Spectroscopic Nanoscopy of Solids**

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Near-field optical microscopy by scattering from an AFM tip, s-SNOM, returns local optical constants from a tiny volume of only  $(20 \text{ nm})^3$  under the tip apex.[1] This enables an extraordinarily high 20-nm optical resolution mapping at any frequency in the VIS, IR, and even THz spectral regions.

The mid-infrared is ideal for nanoscale chemical recognition by vibrational and phonon contrasts. Highlights will be presented of finding and characterizing natural nanoscale inhomogeneities, chemical as well as structural, in organic solar-conversion film,[2] in bone/shell biomineral matter,[3] and in slices through a cometary dust particle.[4]

In solid-state physics, the infrared scattering from the tip can contribute high momenta needed for the excitation of slow surface waves. This unique ability has made s-SNOM surface-plasmon interferometry a unique characterization method of mobile carriers in graphene[5] and BN.[6]

Our development of a coherent IR continuum source[7] has enabled to observe broadband infrared spectra at each image pixel, a method named nano-FTIR. Note both amplitude and phase spectra are recorded. Because the technique uses 100-fs pulses the extension to perform s-SNOM and nano-FTIR with ultrafast time resolution has been straightforward; it has allowed the pump-probe determination of hot carrier dynamics of graphene as well as of bulk semiconductors.[8]

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**#056 - Ultrafast nanoscopy of nanowire surfaces with sub-cycle temporal resolution**

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Ultrafast spectroscopy of materials in the terahertz to multi-terahertz range provides the unique opportunity to study photoinduced dynamics on the sub-cycle time scale. Moreover, this spectral range contains a host of important collective excitations in condensed matter systems, including plasmons, phonons and magnons. Both the dynamics and character of these low-energy excitations can change significantly as the dimensions of a system are reduced to the nanoscale. Their properties can also vary between different nanoparticles in an ensemble, as nanoparticle size, structure, and orientation is often heterogeneous. Direct, ultrafast measurements within single nanoparticles are thus of great interest. Infrared microscopy of surfaces based on near-field scattering can provide a window into this drastically subwavelength world, enabling access to nanoparticle surfaces with 10 nm spatial resolution. Ultrafast, and even sub-cycle, nanoscopy can thus be achieved by combining cutting edge ultrafast and imaging technologies.

Here, we demonstrate a unique combination of ultrafast multi-terahertz spectroscopy with scattering-type near-field scanning optical microscopy (s-NSOM). Phase-stable multi-terahertz pulses are coupled to the tip of an s-NSOM and the scattered radiation is detected by electro-optic sampling. We record the oscillating electric near field with a time resolution given by the duration of the electro-optic gate pulse (10 fs, sub-cycle), while the radius of curvature of the s-NSOM tip apex defines our nano-spectroscopy spatial resolution (10 nm in all three spatial dimensions).

We have applied our novel microscope to the study of ultrafast local carrier dynamics at the surface of an indium arsenide nanowire. Ultrafast imaging of the scattered near-field intensity provides a map of the photoinduced carrier density, while field-resolved nano-spectroscopy reveals its local evolution with sub-cycle time resolution. Tuning our probing depth, we also perform femtosecond tomography and directly resolve the ultrafast (<50 fs) formation of a carrier depletion layer. Finally, as an outlook,

recent measurements on nanowires made of a correlated electron material will be presented to highlight the unique insight that can be gained from ultrafast multi-terahertz nanoscopy.

### #057 - Localized Surface Polaritons in J-Aggregate Nanostructures

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When light interacts with metal nanoparticles and nanostructures, it can excite collective oscillations known as localized surface plasmons (LSPs) which provide the opportunity to confine light to very small dimensions below the diffraction limit [1].

This high confinement can lead to a striking near-field enhancement which can be exploited in sensing and nanophotonics.

Only materials with a negative real part of the dielectric function and moderate losses, are able to excite localized surface waves and hence to confine light to very small dimensions below the diffraction limit. Collective oscillations of free electrons are not the only way a negative permittivity may arise. It may also occur in the high energy tail of a strong absorption resonance [2,3].

We present accurate scattering calculations showing that nanostructures obtained from thin films of J-aggregate dyes [4], despite their insulating behavior, are able to concentrate the electromagnetic field at optical frequencies below the diffraction limit, analogously to metallic nanoparticles. These results, in view also of the huge variety of organic dyes that can aggregate and their chemical flexibility, hold the promise to greatly enlarge the availability of plasmonic materials with different properties with respect to noble metals. For example J-aggregates display attractive nonlinear optical properties which could be exploited for the realization of switchable LSRs for nanophotonic devices.

Specifically we investigate ultrathin nanodisks and nanodisk dimers which can be obtained by nanolithography and nanopatterning techniques. J-aggregate nanoantennas can represent a low-cost solution for improving photovoltaic devices and for the realization of efficient artificial photosynthetic light-harvesting antennas.

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### #058 - Room temperature Terahertz detection with 1D and 2D nanomaterials

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We report on the development of one dimensional (1D) or bi-dimensional (2D) field effect transistors (FETs) based on semiconductor nanowires (NWs) or 2D nanomaterials, as a low-noise, high speed, and high efficiency detection technology across the terahertz (THz) band. Our strategy is based on the possibility to exploit the rectification of the incoming electromagnetic field by hydrodynamic nonlinearities in the FET channel. Terahertz radiation, coupled between the gate (G) and source (S) electrodes, induces an AC field, exciting carrier density oscillations. These oscillations, referred to as plasma-waves<sup>1</sup>, generate a driving longitudinal electric field through the channel. If this simultaneous modulation of carrier density and drift velocity occurs in an asymmetric structure, a DC voltage signal, whose amplitude is proportional to the intensity of the incoming radiation, results at the drain (D) electrode. The required asymmetry can be provided by shaping the S (source) and D electrodes differently<sup>2</sup>, by driving a current through the device, or by realizing an inherently asymmetric channel playing with material morphology, composition, or doping.<sup>3</sup>

A semiconductor NW is ideal to build specific functionalities in a FET: NWs can be assembled with specific compositions, heterojunctions and architectures, promising advanced performance at dimensions compatible with on-chip technologies. Here we report on our recent progresses in the development of 1D InAs or InAs/InSb NW-based FETs exploiting novel morphologies and/or material combinations.<sup>4</sup>

By employing homogeneous InAs NWs we have demonstrated THz detection in the 0.3 THz – 3 THz range with noise equivalent power (NEP) as low as 100 pW/√Hz. Moreover, exploiting the axial asymmetries of tapered gradient-doped InAs NWs and heterostructured InAs/InSb NWs, we developed detectors that can be operated in a gateless configuration, with only a single terminal for the rectified signal readout. This opens a promising possibility for the realization of a compact, multiple-pixel, detection and imaging system.

Furthermore, we have recently studied the application of plasma-wave FET THz detectors based on novel intriguing 2D materials, like exfoliated black phosphorus and three-dimensional topological insulators (TIs) exploiting bismuth compounds. These materials have achieved good detection performances in the 0.26 THz – 0.38 THz range and have been already exploited in a realistic setting for imaging applications.

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### #059 - Core/shell dielectric colloids and metal/dielectric nanostructures: multi-purpose platforms for photon management at the nanoscale

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Core/shell nanostructures are intensively investigated for broadband light trapping and management, because they can play as optical cavities and directly take advantage of morphology dependent resonances. The same properties can be exploited in imaging and vibrational spectroscopy (Raman, IR), in order to enhance their analytical sensitivity. [1-3] Moreover, the synergistic combination of plasmonic nanoantennas and dielectric core/shell colloids allows the fabrication of near-field optical light concentrators. These structures hold great promise in a variety of applications, which can take advantage from a carefully engineered photon management. [4]

This presentation will review some applications of core/shell light nanoconcentrators as non-plasmonic Raman enhancers, which have been used to investigate biochemical reactions, and their coupling to plasmonic nanoantennas for promoting light-assisted chemical reactions.[1-6] Using both approximated analytical models and full wave numerical simulations, the role of morphology dependent optical resonances in driving the spectral response of different systems will be discussed. Finally, the influence of the nonlinear optical properties of the metallic nanostructures on the system optical response is analysed. [7-8]

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### #060 - Gate-controlled plasmonics in single nanostructures

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Nanoplasmonics is emerging as a powerful tool for modern information and communication technologies, as suggested by the recent realization of gate-tunable plasmons in graphene nanostructures [1].

Here we demonstrate that a similar approach can be also very useful for the spatially resolved investigation of fundamental properties of nanostructures. In the present implementation we achieve field-effect control of the plasma resonance in InAs nanowire (NW) devices, detected by scattering-type scanning near-field optical microscopy (s-SNOM) in the mid-infrared region ( $\lambda \sim 10.5 \mu\text{m}$ ) [2].

The NWs are grown with a linearly graded doping which modulates the free carrier axial density, and are deposited on a substrate consisting of 300 nm thick thermal SiO<sub>2</sub> grown on top of bulk n-doped silicon. Optical nano-imaging of individual NWs shows a typical resonant feature that mirrors the axial doping profile. Electrical contacts are fabricated on the NWs while the doped silicon acts as a back gate.

Keeping the NW grounded by the contact electrode, we apply a dc voltage to the substrate and simultaneously probe the plasma resonance along the NW. Using a back-gate voltage in the range (-100,+100)V we detect a 0.75nm/V shift of the axial position of the plasma resonance, induced by the modification of the free carrier density in the NW due to the field effect. Moreover, we implement a setup for low-noise local measurements of the field effect on the carrier density in the NW. From the analysis of our results we are able to extract quantitative information on the electron mobility around the plasma resonance. Our approach leads to the experimental evaluation of key electrical parameters with 20 nm spatial resolution using a non-invasive, all-optical method.

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### #061 - Three-Dimensional Nanohelices for Chiral Photonics at Visible Frequencies

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Chiral Photonics<sup>1</sup> and Chiral Plasmonics<sup>2</sup> are recently emerging fields of research, based on the study and the tailoring of optical effects in chiral metamaterials where incident light and dielectric or metallic structures are arranged in a geometrical configuration lacking of mirror symmetry. The optical response of these systems shows large sensitivity to the circular polarization state of incident light, and this feature can be exploited for applications in optoelectronic devices, integrated quantum optics, or circular dichroism spectroscopy for bio-detection. In this work, we will focus on our recent results about the nanoscale fabrication and the optical investigation of helical metamaterials<sup>3-5</sup>, where extrusion along the vertical dimension and controllable geometrical parameter shrinkage allow the observation of a number of pronounced chiroptical effects in the optical frequency range.

Here we will discuss chiral metamaterials consisting of arrays of three-dimensional helicoidal nanostructures realized by platinum deposition induced by focused ion beam or focused electron beam. The capabilities of this technology have been investigated, with respect to resolution limits, 3D growth control in complex geometries and 3D proximity effects as a function of the interactions between writing beam and deposition environment<sup>3-4</sup>. Arrays of helical nanowires can be accurately engineered to get circular dichroism in different spectral ranges, from NIR to VIS, with highly selective transmission of light handedness. By suitably exploiting the insight in the technological issues affecting the growth of 3D nanohelices, complex intertwined chiral structures, such as Triple-Helical Nanowires, have been realized<sup>5</sup>, allowing the simultaneous observation of multiple chiroptical effects, namely, strong broadband circular dichroism, high circular polarization conversion purity and optical activity, all in the visible range of the electromagnetic spectrum. These three dimensional nanostructures show up to 37% of circular dichroism in a broad range (500–1,000 nm), with a high signal-to-noise ratio (up to 24 dB). Optical activity of up to 8° only due to the circular birefringence is also shown, tracing the way towards chiral photonic devices that can be integrated in optical nanocircuits to modulate the visible light polarization. The experimental results are interpreted as a results of the mutual interaction between surface plasmon modes excited by incident light in individual helical nanowires arranged in close proximity (~100 nm), leading to coupling and hybridization between the plasmon modes, in turn responsible for the broader region of circular dichroism selectivity in the transmission spectra.

### #062 - Pushing the high-energy limit of plasmonics

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The localized surface plasmon (LSP) resonance of metal nanoparticles allows confining the electromagnetic field in nanosized volumes, creating high-field "hot spots", most useful for a huge variety of applications in optics and photonics.

The most commonly employed plasmonic metals, Au and Ag, are upward limited in their LSP energy below the near-UV, due to the strong damping exerted by interband transitions. Pushing the high energy limit of plasmonics to the deep-ultraviolet therefore requires the exploitation of different metals. Without resorting to exotic or expensive materials, it was shown that it is theoretically possible to achieve deep-ultraviolet (DUV) LSP resonances employing one of the cheapest and most abundant materials available on earth: aluminum [1].

Whereas this material would represent a breakthrough in terms costs, two main disrupting factors have stood in the way of practically exploiting Al and achieving the ultimate DUV limit: the first is the strong size-dependence of Al plasmons, calling for ultrafine particles, and the second is the notorious reactivity of Al, leading to its fast oxidation and consequent LSP redshift. These obstacles, though hard, can be however circumvented, employing careful nanofabrication methods and operating under ultra-controlled environment.

In this contribution, we report the successful realization Al NPs with ultrafine size (diameter  $D < 20$  nm) and completely free from superficial oxide. Such particles exhibit indeed a striking high-energy plasmon resonance at 6.8 eV photon energy, the highest energy reported for a LSP [2], that finally approaches the theoretical highest energy.

Since ultra-controlled environments hardly suit applications, we then monitored the effects of a realistic operating environment on the LSP resonance. Controlled exposure of the nanoparticles to a reactive atmosphere showed a gradual surface oxidation and the formation of the well-known passivating oxide layer, causing a general redshift of the LSP to 5.8 eV, still within the DUV range.

However, whereas aluminum nanoparticles of sufficiently large size successfully preserved a sizeable DUV plasmon response when exposed to atmosphere [3], the smallest particles ( $D < 10$  nm) suffered an apparent loss of plasmonic functionality. High-resolution electron spectroscopy investigations allowed to ascribe this effect to a disruption of the metal core occurring during the oxide formation, as the different mobility of anions and cations in the surface region leaves behind vacancy clusters at the oxide-metal interface that eventually coalesce to form hollow nanoparticles for the smallest metal cores [4]. This might represent an intrinsic upward limit for Al plasmonics under atmospheric operating conditions.

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-

**#063 - High-order harmonic generation in intense laser field and Fano resonances**

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Other Authors: M. Khokhlova (M.V. Lomonosov Moscow State University, Moscow, Russia)

Using the resonances of the generating medium is a natural way to boost the high-order harmonic generation (HHG) efficiency. Generation of high harmonics with frequencies close to that of the transition from the ground to an autoionizing state (AIS) of the generating particle were experimentally investigated in plasma media [1] and in noble gases.

A number of HHG theories based on the specific properties of AIS were developed. These theories involve three-step rescattering model [2] in which the HHG is described as a result of tunneling ionization, classical free electronic motion in the laser field, and recombination accompanied by the XUV emission upon the electron's return to the parent ion. In particular, in Ref. [3] one of us suggested a four-step resonant HHG model. The first two steps are the same as in the three-step model, but instead of the last step (radiative recombination from the continuum to the ground state) the free electron is trapped by the parent ion, so that the system (parent ion + electron) lands in the AIS, and then it relaxes to the ground state emitting XUV.

We develop the HHG theory considering AIS in addition to the ground state and free continuum treated in the theory [4] for the non-resonant case. We show that such accurate consideration verifies the model [3]. The details of our approach are presented in [5]. We find that the spectrum of the dipole moment of the system is the product of the Fano-like factor and the harmonic line which would be emitted in the absence of the AIS. Our theory allows calculating not only the resonant harmonic intensity, but also its phase. We show that there is a rapid variation of the phase in the vicinity of the resonance. Our calculations reasonably agree with recent harmonic phase measurements [6].

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**#064 - Ultrafast photo-physics and photo-chemistry for model systems of biomolecule interactions**

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Understanding and tagging interactions between biomolecules has become one of the most crucial tasks of modern life sciences with enormous fallouts in all scientific fields. To this end a number of models have been proposed in a reductionist approach, to mimic a simplified "hot core" of an interaction between molecules having very complicated structures. 5-Benzyl Uracil (5BU) was originally proposed as a model system for the nucleic acid – protein interactions at a molecular level. In particular, it was selected as a model for better understanding the interaction between nucleic acid and proteins in a reductionist view as containing functional group analogs of nucleic acids and/or amino acids identified as photo-reactive in the literature. Additionally, 5BU undergoes clean intramolecular photo-cyclization when irradiated with UV light (250 – 260 nm). Studying the rich ultrafast photo-physics and photo-chemistry of this model system retrieved by an accurate spectroscopic investigation, can lead to gain insights both in the ultrafast processes involved in the photo-cyclization process and in nucleic acid - protein interactions. Moreover, since for 5BU the presence or absence of oxygen does not modify the photo-cyclization quantum yield, this suggests that the occurring crosslinking reaction involves singlet state chemistry and their ultrafast dynamics.

Excited states decay times of 5BU are estimated in the tens of picoseconds timescale and, since 5BU photochemistry involves the dynamics of a ring closure which is investigated to realize molecular switches, studying the ultrafast processes triggered in such a system promises to imply great progresses with noticeable practical applications. In particular, we report the ultrafast fluorescence decay investigation of the molecule in response to a femtosecond UV exciting pulse, obtained by means of a fluorescence up-conversion setup with high temporal resolution and with a spectral response extended down to the deep UV range.

5BU dynamics is expected to be considerably affected by the solvent, as observed for the nucleobases and in particular for Uracil, which was found to have a different decay when passing from gas phase to methanol. Thus, we also carried on an investigation of the role played by the solvent by characterizing the different steady-state absorption spectrum of the photo-cyclized product in water and methanol. Being this response very much different we can, then, infer that water is favoring photo-cyclization, what could have very crucial consequences also in better understanding the role played by the water molecule present in the intracellular medium when looking at 5BU as a model of nucleic acid protein interactions.

**#065 - High-energy recollision processes in strong-field QED**

Antonino Di Piazza - Max Planck Institute for Nuclear Physics

Two oppositely charged particles created within a microscopic space-time region can be separated, accelerated over a much larger distance, and brought to a



recollision by a laser field. Consequently, new reactions become feasible, where the energy absorbed by the particles is efficiently released. By investigating the laser-dressed polarization operator, we identify a new contribution describing high-energy recollisions experienced by an electron-positron pair generated by pure light when a gamma photon impinges on an intense, linearly polarized laser pulse [1]. The energy absorbed in the recollision process over the macroscopic laser wavelength corresponds to a large number of laser photons and can be exploited to prime high-energy reactions. Thus, the recollision contribution to the polarization operator differs qualitatively and quantitatively from the well-known one, describing the annihilation of an electron-positron pair within the microscopic formation region [2].

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#### #066 - Controlling photoemission from laser-driven quantum rings

*Pietro Paolo Corso - Università degli Studi di Palermo - Dipartimento di Fisica e Chimica*

The diffused radiation from planar and structured quantum rings driven by an intense laser field is investigated. Adopting all the possible simplifications that do not hide the essential effects, the time dependent Schroedinger equation is numerically solved by considering a single active electron. We investigate the characterization of the emitted radiation as a function of some parameters concerning the geometry of the system and the laser polarization. The results show that manipulation of these parameters provides important handles to control the emitted spectrum indicating that the investigated systems are efficient sources of radiation.

#### #067 - Angular-resolved photoelectron spectroscopy of many-electron systems from a time-dependent density-functional theory perspective

*Umberto De Giovannini - University of the Basque Country EHU/UPV*

Photoelectron spectroscopy is a technique widely used to study the electronic properties of a large variety of physical systems ranging from atoms and molecules to solids and surfaces. Electrons ejected from these systems carry a wealth of information on the parent ions and the ionization process which is encoded in the angular distribution of their velocities. Analyzing the data to extract physical information with simple analytical tools is only possible under very specific conditions. Recent advances in the development of intense and/or ultra-short light sources offer new opportunities to study exotic and highly excited states also as a function of time [1] whose analysis require theoretical tools way beyond the simple analytical ones. Building an ab-initio approach to model these kind of process is a difficult task since it requires to deal with infinitely extended states of many-electron systems in the presence of time-dependent external fields.

Time-dependent density functional theory (TDDFT) offers a simple yet powerful framework to describe many-electron systems interacting with external electromagnetic fields. The simplicity resides in the mapping of the complicated many-body problem onto a problem of non-interacting electrons in the presence of an effective time-dependent single-particle potential. The theory is formally exact and in principle can give access to the exact time-dependent density of an interacting system.

We present a method, based on a geometrical partitioning scheme that efficiently can give access to momentum-resolved photoelectron spectra of multi-electron systems within TDDFT [2]. We introduce the theory and illustrate the core algorithms applicable to real-space real-time formulations. We show how this techniques can be easily extended to study time-resolved pump-probe experiments in which a system response (electron emission) to a probe pulse, is measured in an excited state [3]. This simulation tool can help to interpret attosecond time-resolved spectroscopic experiments, where the electronic motion must be followed at its natural time-scale. Further, by including the ionic motion, we show how this approach can provide direct insight into molecular photochemical reactions [4] and discuss under which conditions it is possible to reconstruct the molecular orbitals from the photoelectron angular distribution [5].

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#### #068 - Quantum breathing frequency of a harmonically trapped quantum gas

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We present an explicit formula for the quantum breathing frequency  $\omega_b$  of a harmonically trapped quantum gas with inverse power-law repulsion. We show how it is possible to express the average values of some important observables of the trapped quantum gas as a function of the breathing frequency. It is therefore argued that measurements of  $\omega_b$  can accurately describe the state of harmonically trapped interacting particles. The formula for  $\omega_b$  is confirmed by numerical calculations for a system of electrons confined in a lateral (2D) quantum dot.

#### #069 - Efficient attosecond pulse generation from HHG spectra

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In this work we propose a method to obtain a single attosecond pulse through the manipulation of the HHG spectra emitted from simple systems driven by an intense laser field. In particular, by means of suitable frequency shift of the emitted radiation followed by subsequent pulses recombination, we show that it is possible the generation of ultrabroadband "quasi-continua" spectra leading to an isolated attosecond pulse. The importance of this technique lies in the possibility of using laser sources which are commonly available in most laboratories.

# September 29

Computational Biophysics II	Gianluca Lattanzi
Interdisciplinary statistical physics.	Raffaella Burioni
From nanoparticles to nanostructured surfaces	Marco Bernasconi
Plasma Physics II	Giovanni Peres
Magnetism and Spin related phenomena II	Marco Affronte
Iron Based Superconductors	Pietro Carretta
Oxide Films and Interfaces	Marco Finazzi
Sustainable Nanotechnologies II	Antonio Martorana
Quantum Fluctuations and Casimir Forces	Roberto Passante
2D emerging materials I	Andrea Tomadin
Nanophotonics II	Dario Pisignano
THz and Quantum Cascade Lasers	Gaetano Scamarcio
Computational Biophysics III	Alessandro Laio
Diffusion and reaction in complex systems	Giuseppe Gonnella
Noncovalent interactions: advances in Computer Simulations	Pierluigi Silvestrelli
Plasma Physics III	Francesco Pegoraro
Magnetism and Spin related phenomena IV	Lucia Sorba
Optical bio-sensing	Francesco Baldini
3d and 5d TM systems	Mario Cuoco
Sustainable Nanotechnologies III	Dario Duca
Photovoltaic materials and devices	Francesco Priolo
2D emerging materials II	Camilla Coletti
Optofluidics	Pietro Ferraro

**#070 - Clustering by search-and-find of density peak: a cheap and unsupervised approach to map complex data landscapes.**

Alessandro Laio (I) - SISSA

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Cluster analysis is aimed at classifying elements into categories on the basis of their similarity. Its applications range from astronomy to bioinformatics, bibliometrics, and pattern recognition. We propose an approach based on the idea that cluster centers are characterized by a higher density than their neighbors and by a relatively large distance from points with higher densities. This idea forms the basis of a clustering procedure in which the number of clusters arises intuitively, outliers are automatically spotted and excluded from the analysis, and clusters are recognized regardless of their shape and of the dimensionality of the space in which they are embedded [Science, vol 344, p. 1492 (2014)]. We will describe applications of this approach to molecular modeling, bioinformatics and neuroimaging.

**#071 - Exploring the Molecular Mechanisms of Photosynthesis by Ab Initio Molecular Dynamics**

Leonardo Guidoni (I) - Università dell'Aquila

The understanding of the molecular mechanisms and the catalytic strategies photosynthetic proteins in plants, algae and cyanobacteria offers many challenges to theoretical biophysicists. These mechanisms include the capture of light by antenna systems, the primary charge separation that convert the photon energy into chemical energy, and the subsequent cascade of biochemical processes leading to the formation of stable high-energy organic products that can be stored in the living organisms. One fundamental step of such mechanisms is the conversion of the electronic excitations into chemical energy used to perform the light-driven transformation of water molecules into molecular oxygen and hydrogen equivalents, i.e. water splitting. This reaction occurs through a series of intermediate steps S0-S4 of the so-called Kok-Joliot's cycle in the Oxygen Evolving Center of Photosystem II (PSII), recently crystallised at atomic resolution [1]. Beyond their interests in biophysics, the comprehension of photosynthetic water splitting mechanisms may also inspire artificial devices [2,3].

By means of Quantum Mechanics / Molecular Mechanics (QM/MM) calculations, we were able to rationalize previously puzzling experiment [4,5] and to understand the complex proton-coupled-electron-transfer mechanisms along the way to water splitting [6]. In the present contribution I will focus mainly on the very early events following the first charge separation which is occurring in the so-called P680 complex, a tetramer of four chlorophylls having a twofold pseudo-symmetry. The photo-induced electron transfer is supposed to leave an oxidising hole shared between two particular chlorophylls, P<sub>D1</sub> and P<sub>D2</sub>, which form the so-called "special pair" of chlorophylls of PSII. This oxidised, charged, pair of chlorophylls is known to be stable for about a hundred of ns before in turn it oxidizes in normal conditions one of the two pseudo-symmetric tyrosines nearby, Tyr<sub>2</sub>[7]. Using QM/MM ab initio molecular dynamics we have detected an asymmetry in the charge distribution of the oxidised special pair, in agreement with several experiments. We have also characterised the origin and the dynamics of this asymmetry, pointing out the key role of the mutual orientation of the chlorophylls and of the protein environment.

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**#072 - Step by step: gold nanoparticles enter biomembranes**

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Other Authors: Federica Simonelli, Davide Bochicchio and Riccardo Ferrando Physics Department, University of Genoa, Italy

Metal nanoparticles (NP) play more and more important roles in pharmaceutical and medical technology as diagnostic or therapeutic devices. Metal NPs can nowadays be engineered in a multitude of shapes, sizes and compositions, and they can be decorated with an almost infinite variety of functionalities. Despite such technological advances, there is still poor understanding of the molecular processes that drive the interactions of metal NPs with cells. Cell membranes are the first barrier encountered by NPs entering living organisms. The understanding and control of the interaction of nanoparticles with biological membranes is therefore of paramount importance to understand the molecular basis of the NP biological effects.

Here we address, by means of coarse-grained Molecular Dynamics simulations, the interaction of ligand-protected Au NPs with model phospholipid membranes. We elucidate the molecular mechanisms involved during the passive membrane permeation and identify the most favorable structural arrangements of the NP-membrane complex. We compare NPs with different ligand compositions, and study their interaction with lipid membranes as varying their degree of hydrophobicity, surface pattern and surface charge.

**#073 - Designing highly specific probes with tunable affinity**

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Finding ligands able to bind with high specificity and tunable affinity to a target protein is one of the major challenges in medical research[1]. To this aim we develop a computational protocol based on the coarse-grained protein model "Caterpillar" [2] that has proven to be quantitative for design and folding simulations. We apply the model to design proteins that bind specifically to a simple pocket. The generated pocket specific sequences can be tuned with different binding free energies, computed using the Caterpillar and verified with all atom MD simulations.

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[2] PloS one, 6(7), e20853. (2011)

**#074 - Multiple binding modes of ibuprofen in human serum albumin identified by alchemical free energy calculations**

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Other Authors: Stefania Evoli (Department of Physics, University of Calabria, Rende, Italy), Rita Guzzi (Department of Physics and CNISM Unit, University of Calabria, Rende, Italy), David L. Mobley (Departments of Pharmaceutical Sciences and Chemistry, University of California, Irvine, United States of America)

Human serum albumin (HSA) is the most abundant protein in blood plasma, where it transports a wide range of ligands including fatty acids, drugs and metabolites. Ibuprofen is a pharmaceutical compound widely used for its anti-inflammatory effects and to control or reduce pain and fever. It is almost insoluble in water and, when administered in ordinary quantities, is almost entirely carried by albumin in the blood. A complete map of the binding of ibuprofen to HSA is complicated to obtain in 'wet lab' experiments, for at least two reasons. First, albumin has multiple binding sites available to accommodate small ligands. Second, ibuprofen may occur either in a charged or neutral form, as well as in two enantiomers with different therapeutic activity.

In this work, by using a combination of molecular docking, molecular dynamics (MD) simulations and alchemical free energy calculations, we report an accurate prediction of the geometry, protonation state and affinity of binding for the pharmaceutically most active form of ibuprofen to HSA. In particular, molecular docking was employed for a large screen of the protein surface in search of binding poses, which were subsequently simulated in conventional MD runs. Binding modes showing a stable placement were selected by using clustering analysis techniques, on the basis of their position, interaction energy and other factors. Finally, absolute binding free energy calculations were used to estimate the binding affinity.

The results show that Sudlow's drug site 2 (DS2) is the preferred binding site for the charged S- enantiomer of ibuprofen in HSA, with a very favorable binding free energy,  $-18.0 \pm 0.6$  kcal/mol. Two other high affinity sites are predicted to correspond to Sudlow's drug site 1 (DS1) and the fatty acid site 6 (FA6), with binding affinities in the range from  $-10.4$  to  $-15.4$  kcal/mol. In contrast, less favorable values of the binding free energy were found for ibuprofen bound in the other fatty acid sites, as well as in the protein cleft in between subdomains IB-IIIa. For ibuprofen in neutral form, the free energy of binding is drastically less favorable (by at least 4.0 kcal/mol), ruling out the possibility that the ligand is protonated within the protein matrix.

These findings provide a detailed description of the binding of ibuprofen in HSA, and may help to explain a wide range of experimental results reported in the literature and obtained with several different techniques.

**#075 - Minimum Valence Principle. Design of natural, artificial and bionic proteins**

Ivan Coluzza - University of Vienna

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Self-assembling is the process by which a substance spontaneously reaches a specific long-lived configuration with a well-defined structure. Such structures may be highly inhomogeneous but still strongly differ from random amorphous materials, which are typically dynamically arrested. In fact by having an easily accessible ground state, self-assembling materials have the property of forming structures characterized by few defects, and they often have the capacity to adapt to changes in the environment. In nature proteins are an extraordinary example of self-assembling material. Proteins have two key features: they are all made of sequences of only 20 chemically different blocks, their functions and structures are precisely controlled by the sequence of amino acids. All life that we know of is built upon these elements. In this presentation I will show two breakthrough results that sprouted from the understanding of how the protein features can be transferred to an artificial system that we refer to as Bionic Proteins [1-2].

The Caterpillar protein model [3-4] demonstrated that quantitative protein design and folding could be achieved with a model that qualitatively captured the valence of the protein backbone interactions. Many examples demonstrated the power of the model to predict the folded structures of natural proteins as well as produce realistic completely artificial sequences for again natural proteins.

Bionic proteins are chains of colloidal particles each covered by a chemical layer that gives them different flavors mimicking the amino acids. In addition to the layer each particle is decorated with spots that create a strong preference for specific particle-particle relative orientations. These two elements were enough to allow the design sequences that would self-assemble in a large spectrum of target structures including knotted chains which have important application for drug design.

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#### **#076 - Intermolecular interaction and diffusion in fibril-forming protein solution: Beyond the colloidal approach**

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The role of intermolecular interaction in fibril-forming protein solutions and its relation with molecular conformation is a crucial aspect for the control and inhibition of amyloid structures. We have investigated protein-protein interactions for different fibril-forming proteins (lysozyme, insulin,  $\alpha$ -chymotrypsinogen) by small-angle neutron and x-ray scattering, measuring the static structure factor, and by static and dynamic light scattering, measuring the second virial coefficient and the Kirkwood-Buff integral. The latter allowed us to take into account the role of density fluctuations even at high concentrations and to show that electrostatic interactions are the dominant contribution for colloidal interactions in the studied protein solutions. As protein concentration increases, the strength of protein-protein interactions decreases, with a more pronounced decrease at low salt concentrations. Such effective "crowding" is due to the long-ranged electrostatic repulsions that are prominent even at moderate protein concentrations (Blanco et al. *J. Phys. Chem. B* 2014, 118, 5817-5831, Blanco et al. in preparation). The crowding effects were confirmed and quantified by assessing the hydrodynamic factor and the protein collective and self-diffusion by using photon and fluorescence correlation spectroscopy. Both techniques evidence how an increase of concentration hinders protein self-diffusion, likely due to both hydrodynamics and crowding effect (Raccosta et al. in preparation). Moreover, we have investigated the relation between intermolecular interaction and protein conformational stability. In the case of lysozyme, proteins are driven out of metastability through conformational sub-states, which are kinetically populated and experience lower activation energy for fibril formation. This explains how electrostatic repulsion may act as a gatekeeper in selecting the appropriate pathway to fibrillation (Raccosta et al. *J. Phys. Chem. B* 2012, 116, 12078-12087).

**#077 - Quasi-stationary states in particle systems with power law interactions**

*Michael Joyce (I) - Université Pierre et Marie Curie - Paris 6*

Quasi-stationary states" are very long lived non-equilibrium stationary states which have been observed in numerous classical many body systems with long-range interactions. I will first review the nature of these states and their theoretical interpretation within the framework of the Vlasov equation. In the rest of the talk I will address the question of how their existence is tied to the nature of the underlying interaction, and in particular to its properties at large and small scales.

Two quite different approaches to the question lead to the conclusion, born out by numerical study, that the existence of these states is a robust property only for interactions for which the pair force is non-integrable at large separation. This motivates a natural classification of interactions into "dynamically" long/short range which is distinct from the usual thermodynamic classification.

**#078 - Estimating topological properties of weighted networks from limited information: applications to socio-economic field**

*Andrea Gabrielli (I) - Istituto dei Sistemi Complessi (ISC) - CNR*

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A problem typically encountered when studying complex systems is the limitedness of the information available on their topology, which hinders our understanding of their structure and of the dynamical processes taking place on them. A paramount example is provided by financial networks, whose data are privacy-protected: banks publicly disclose only their aggregate exposure towards other banks, keeping individual exposures towards each single bank secret. Yet, the estimation of systemic risk strongly depends on the detailed structure of the interbank network. The resulting challenge is that of using aggregate information to statistically reconstruct a network and correctly predict its higher-order properties. Standard approaches either generate unrealistically dense networks, or fail to reproduce the observed topology by assigning homogeneous link weights. Here we develop an improved reconstruction method based on statistical mechanics concepts, that makes use of the empirical link density in a highly nontrivial way. Technically, the novelty of our approach lies in the preliminary estimation of node degrees from empirical node strengths and link density, followed by a maximum-entropy inference based on the combination of empirical strengths and estimated degrees. Our method is successfully tested on the international trade network and the interbank money market, and represents a valuable tool for gaining insights on privacy-protected or partially-accessible systems.

**#079 - Kuramoto model of synchronization: equilibrium and nonequilibrium aspects**

*Stefano Ruffo (I) - Dipartimento di Fisica e Astronomia Università degli Studi di Firenze*

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Recently, there has been considerable interest in the study of spontaneous synchronization, particularly within the framework of the Kuramoto model. The model comprises oscillators with distributed natural frequencies interacting through a mean-field coupling, and serves as a paradigm to study synchronization. In this talk, I will describe the model from a different point of view, emphasizing the equilibrium and nonequilibrium aspects of its dynamics from a statistical physics perspective. I will discuss in a unified way known results with more recent developments obtained for a generalized Kuramoto model that includes inertial effects and noise.

**#080 - The Scientific Competitiveness of Nations**

*Giulio Cimini (I) - Istituto dei Sistemi Complessi (ISC-CNR) UoS "Sapienza" Università di Roma*

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We use citation data of scientific articles produced by individual nations in different scientific domains to determine the structure and efficiency of national research systems. We characterize the scientific fitness of each nation---that is, the competitiveness of its

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research system---and the complexity of each scientific domain by means of a non-linear iterative algorithm able to assess quantitatively the advantage of scientific diversification. We find that technological leading nations, beyond having the largest production of scientific papers and the largest number of citations, do not specialize in a few scientific domains. Rather, they diversify as much as possible their research system. On the other side, less developed nations are competitive only in scientific domains where also many other nations are present. Diversification thus represents the key element that correlates with scientific and technological competitiveness. A remarkable implication of this structure of the scientific competition is that the scientific domains playing the role of "markers" of national scientific competitiveness are those not necessarily of high technological requirements, but rather addressing the most "sophisticated" needs of the society.

#### **#081 - Glassy photonics: statistical mechanics and replica symmetry breaking in lasing in random media**

*Luca Leuzzi - CNR-NANOTEC, Soft and Living Matter Lab., Rome*

*Other Authors: Fabrizio Antenucci, CNR-NANOTEC, Soft and Living Matter Lab., Rome; Andrea Crisanti, Sapienza University, Rome*

The behavior of a newly introduced overlap parameter is analyzed, measuring the correlation between intensity fluctuations of waves in random media in different physical regimes, with varying amount of disorder and non-linearity. Its relationship is established to the standard Parisi overlap order parameter in replica theory for spin-glasses. In the complex spherical spin-glass model, describing the onset and behavior of random lasers, replica symmetry breaking in the intensity fluctuation overlap is shown to occur at high pumping or low temperature. This order parameter identifies the laser transition in random media and describes its glassy nature in terms of emission spectra data, the only data so far accessible in random laser measurements. The theoretical analysis is, eventually, compared to recent intensity fluctuation overlap measurements demonstrating the validity of the theory and providing a straightforward interpretation of different spectral behaviors in different random lasers.

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**#082 - Symmetry breaking in core-shell nanoalloys***Riccardo Ferrando (I) - Dipartimento di Chimica e Chimica Industriale dell'Università di Genova*

Nanoalloys are bi- or multi-component metallic particles in the size range between 1 and 100 nm. Nanoalloys present a wide variety of structures and properties, which make them suitable for many applications in catalysis, optics, magnetism and biomedicine. Nanoalloys of weakly miscible metals present core-shell and Janus structures as preferential arrangements. Size- and composition-dependent transitions between these arrangements can be rationalized by a unifying concept, that is symmetry breaking, caused by the accumulation of strain at the atomic level and its subsequent release. Several binary metallic systems, such as Ag-Cu, Ag-Co, Ag-Ni, Au-Co, and Cu-Ni are treated, comparing computational results to experimental observations.

**#083 - From size-selected gold nanoclusters to nanostructured surfaces: solving the atomic structure of model nanoparticles with multiple applications***Richard E Palmer (I) - University of Birmingham*

The controlled deposition of beams of size-selected nanoclusters (nanoparticles), assembled from atoms in the gas phase and mass-selected before deposition, is a novel [1] but increasingly popular route to the fabrication of functional surfaces structured on the sub-10nm scale, with applications in catalysis, coatings, radio-sensitizers and biochips [2]. These systems also have the potential to serve as model, ultraprecise reference materials for bio-imaging and metrology (e.g. cryo-electron tomography) and nanotoxicology. Efforts to scale-up the rate of cluster generation thus promise significant future impact and will be summarised. However fundamental questions remain over the equilibrium atomic structures of the clusters themselves, since direct gas phase structural studies have been limited and new techniques like aberration-corrected scanning transmission electron microscopy (ac-STEM) are only now being applied to soft-landed, size-selected clusters.

I will survey our recently published [2-8] and latest systematic ac-STEM experiments which address the atomic structure of size-selected "magic number" gold clusters – Au<sub>20</sub>, Au<sub>55</sub>, Au<sub>309</sub>, Au<sub>561</sub>, and Au<sub>923</sub> – including dynamical manipulation experiments [6], which probe the transformation of metastable isomers into more stable configurations, and reaction-exposure experiments, which probe the stability of the nanocluster structures under real catalytic conditions. The results distinguish the hierarchy of competing isomers as a function of cluster size, expose concepts such as templated-growth, provide a body of data to stimulate and constrain computational models and are readily extendable to other sizes and cluster materials including binary systems. The image shows one frame from a dynamical STEM video of an Au<sub>923±23</sub> cluster.

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**#084 - Simulating friction of well-characterized deposited 'nano'-systems: from metallic clusters and rare-gas islands to colloidal monolayers***Andrea Vanossi (I) - CNR-IOM DEMOCRITOS & SISSA*

The high complexity of dealing with systems with many degrees of freedom under a strict size confinement arises especially in sliding friction phenomena, where the key mechanisms take place at a buried interface.

In the last three decades, developments in nanotechnology have extended the experimental study of friction, permitting the analysis on well-characterized materials and surfaces at the nano and mesoscale.

Here, by presenting three case studies related to the frictional properties of deposited metallic clusters[1,2], physisorbed rare-gas islands[3,4] and driven colloidal monolayers[5,6], we show how modeling and molecular dynamics simulations may help in advancing our theoretical understanding in the field of nanotribology.

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#### #085 - Au-based molecule-like clusters for enhanced quantum efficiency emission of Er<sup>3+</sup> ions in silica

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Visible and infrared luminescence from rare earth ions (Er, Eu) finds a variety of technological applications, spanning from optical telecommunications, to solar cells and light emitting devices. The excitation cross section is intrinsically low due to the parity-forbidden character of the involved  $f-f$  transitions. Our group recently demonstrated that  $Au_N$  clusters (with  $N=5-20$  atoms) are able to boost the photoluminescence (PL) of  $Er^{3+}$  located in close proximity (few nm) by a non-resonant broad-band pumping scheme, with a resulting enhancement of their effective excitation cross section by 2-3 orders of magnitude with respect to the same system without metal clusters [1].

This paper reports the formation by sequential ion implantation of Au or Au-Ag sub-nanometer alloy clusters in silica and Er-doped silica, and on the effect of their optical properties on the enhanced quantum efficiency of the  $Er^{3+}$  PL. This energy transfer process is demonstrated to depend on the clusters size (as obtained by EXAFS analysis), but also on cluster composition, since it is triggered by the cluster electronic energy level structure. As shown in Fig. 1, with respect to  $Au_N$ , we found that  $(Au_xAg_{1-x})_N$  are remarkably more effective in promoting the  $Er^{3+}$  emission enhancement. This will be correlated in a Förster-type energy transfer scheme to a recently demonstrated PL emission from the metallic nanoclusters themselves [2,3].

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#### #086 - Understanding the catalytic activity of large polyhedral nanoparticles from first-principles

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In the endless search of new green alternatives for energy conversion other than fossil fuels burning, proton exchange membranes fuel cell (PEMFC) play a major role, converting chemical energy into electricity with extremely high efficiency and small impact on the environment. [1] Notwithstanding that platinum is one of the best materials for electrodes, its high price and its low resistance to poisoning motivate the efforts of researchers worldwide in finding possible cheaper substitutes. One way is lessening the amount of Pt reducing its size and mixing it with other elements. Computational modelling can aid experimentalists in understanding at molecular level the processes occurring at the interface between reactants and electrodes. [2] Unfortunately theory and experiments cannot easily find a connection due to the "size gap", where nanocatalysts of 1-100 nm are synthesized in the laboratory, while numerical simulations model nanoparticles in the sub-nm regime and rarely larger than 3 nm. The size gap might be overcome following the roadmap presented here. It implies (i) the recognition of all inequivalent adsorption sites characterizing the real nanocatalysts; (ii) the prediction of how their number varies against nanoparticle size, (iii) the identification of the smallest cluster with all the relevant sites on which perform the study of the reaction profile, and finally (iv) the extrapolation of the behaviour at experimental relevant sizes. Density-functional results obtained on several Pt, Ni and Pt-Ni nanomorphologies, either in the gas phase or deposited on MgO, are reported as a paradigmatic example [3].

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#### #087 - Clusters, Surfaces, Defects in Metal-Ceramic Systems with DFT and Variable Charge Classical Molecular Dynamics

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The study of metal/ceramic interfaces is crucial for the understanding of complex processes such as corrosion and oxidation as well as for applications such as thermal barrier coatings.

At present, the understanding of such processes at an atomistic level, that would be beneficial for different technological applications, is limited to structural analysis.

Atomistic simulations aimed at the investigation of metal/ceramic interfaces face two main problems:

- i) large scale of models needed for a realistic representation of an interface,
- ii) relevance of non-equilibrium processes that require access to long time scales for the simulation of dynamical processes.

Despite ab initio simulations at the DFT level already proved to be successful in this context, to gain insight into the non-equilibrium effects an approach relying on empirical potentials is mandatory. However, the availability of reliable empirical potentials for metal/ceramic systems is restricted to few case studies.

The main problem is that an accurate description of a metal/ceramic interface requires a potential able to account for charge equilibration at the interface and according to the neighbours of each atom.

Recently generic formulations for metallic, ionic and covalent bonding fulfilling the requirement of charge equilibration have been introduced and subject to continuous extensions [1].

Following this trend, we study metal-ceramic systems by means of recently developed potentials [2, 3].

In this work we present preliminary results with focus on  $\text{Al}_x\text{O}_y$ .

Selection of ad hoc structures will allow us to assess the validity of the novel potentials by means of comparison with results based on ab initio simulations.

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#### #088 - Spontaneous oxidation of Ni nanoclusters on MgO monolayers induced by segregation of interfacial oxygen.

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Metal nanoparticles (NP) dispersed or supported on oxide substrates have important applications ranging from nanoelectronics to magnetism, pharmaceuticals (e.g. for biological labeling) and catalysis. It is now well established that the NPs' properties depend critically on their size and shape [1,2]. However, in spite of the large literature on the topic, most of the attention has concentrated so far on metal NP made of a few tens of atoms or more [2]. Relatively few studies, both experimental [3,4] and theoretical [5], have been performed on single atoms or groups of very few atoms supported on insulating surfaces. In these cases, the catalytic activity was shown to be size-dependent and directly related to the intrinsic electronic and geometric properties of the NP.

Considering the technological relevance of these nano-objects, a clear description of their properties also in the very low size limit is important. This is particularly true in the case of Ni, which combines its magnetic nature to a strong catalytic activity.

We show here the results of a combined LT-STM and DFT investigation of the Ni/MgO/Ag(100) system. We take advantage of our ability to grow perfectly flat and extended MgO monolayer films on Ag(100) [6,7], which are an optimal substrate for the deposition of NP. We focus our attention on the smallest Ni NP, up to six Ni atoms in size, and we demonstrate that, at low Ni coverage and  $100 \text{ K} < T < 250 \text{ K}$ , flat structures completely different from the 3D clusters predicted for  $\text{Ni}_4$ ,  $\text{Ni}_5$  and  $\text{Ni}_6$  clusters form [8]. By combining the morphological information deduced by STM images with the outcome of density functional theory calculations, we demonstrate that they consist of  $\text{Ni}_y\text{O}_x$  aggregates. We interpret this result as a consequence of the presence of interface oxygen available immediately below the MgO layer, which segregates to the surface and binds to the reactive Ni atoms. Thus, the latter ones act as pumps to extract oxygen from the substrate. Besides being of interest in view of the different catalytic properties of Ni and  $\text{NiO}_x$ , our results demonstrate once more the peculiarity of ultrathin oxide films with respect to the corresponding bulk materials and suggest that the physics of these systems is still far from being completely understood.

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**#089 - Stochastic Resonance in a Surface Dipole**

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In the case of a neutral dipole, made up of two bound equal pointlike masses (monomers) carrying opposite charges, an external electric field pulls the monomers to opposite directions. The field, no matter whether dc or ac, cannot induce a net dipole current, since the total force applied to the neutral dipole center of mass is zero. As a consequence, the motion of the center of mass on a symmetric substrate is purely diffusive. However, the internal degree of freedom of a dipole, when constrained to 1D and subjected to an oscillating field of force, exhibits interesting properties, which result from the interplay of monomer–substrate and monomer–monomer interactions [1]. Namely, it is observed that the amplitude of the forced oscillations of the dipole can be enhanced by tuning the noise strength, i.e., the substrate temperature. Such a manifestation of stochastic resonance turns out to be extremely sensitive to the mechanical properties of the dipole, i.e., to the length and elasticity of the dipole (see also Ref. [2]), having immediate applications to surface physics and nanotechnology.

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**#090 - Advanced plasma ion sources and beam formation**

Marco Cavenago (I) - INFN-LNL

Ion sources are a basic part of many accelerator systems, with emphasis on different goals, ranging from ion charge state (say  $\text{Xe}^{35+}$  at a current of almost 0.1 mA for Electron Cyclotron Resonance Ion Sources ECRIS) to large currents for the applications of accelerator based neutron production (say 100 mA of  $\text{H}^+$  or  $\text{D}^+$  with a single beam extraction aperture) or of tokamak plasma heating (say 50 A of  $\text{D}^+$  or  $\text{D}^-$  with a necessarily multi-aperture extraction). In most cases, ions are produced into plasmas and diffuse to extraction; so the optimal ion confinement time is a compromise between needs of sustaining the plasma discharge and of increasing current. While quasi-neutrality holds inside plasmas, at their surfaces the formation of sheaths, that are charged plasma layers with the thickness of few Debye lengths, and of presheaths, must be included in any accurate model [Forrester, 1996]. The structure of a sheath depends on the applied magnetic field and the kind of walls, insulating (so that local balance of ion and electron currents to wall is required) or conducting, so only global balance is required [Drentje, 2002]. In any case cold plasma sheath layers follow wall shapes, where wall exists, and form an approximately round shape called "meniscus" at beam extraction aperture. A satisfying focusing of the extracted beam depends on meniscus shape, and it is experimentally obtained by regulating adjustable parameters as the extraction voltage. Ion production optimization depends from the source, and often requires careful engineering to achieve required levels of magnetic fields for confinement, of heating power density and of wall conditioning.

In this presentation only two kinds of plasma ion sources (with microwave or radiofrequency heating) are taken as examples, namely the ECRIS [Geller, 1998] and the radiofrequency heated NIS (Negative Ion Sources) [Fantz, 2008], outlining some of the optimization and technical issues. In the former, the need to achieve a relatively large electron temperature ( $T_e > 1$  keV) at a necessarily low gas pressure ( $< 0.0001$  Pa) has promoted a quest for ever increasing magnetic fields (many T), with a minimum B linear trap configuration, and for UHV conditions. In NIS for fusion application a low electron temperature ( $T_e$  about 1 eV) is required for reducing  $\text{H}^+$  ionization, while a larger temperature (about 4 eV) is required for dissociation of  $\text{H}_2$  and efficient plasma production at reasonable gas pressures (order of 1 Pa and preferably less) and moderate electron densities (order of  $n_e = 10^{18} \text{ m}^{-3}$ ). Plasma cavity is consequently divided into two volumes by a filter magnetic field. Its optimization represents an open issue both for theory and for the engineering, here discussed by simple models. Optimal values usually found in experiments are in the 0.005 T order of size. Other elaborate magnetic field and accelerator electrode configurations needed for electron beam dumping and accurate aiming of the ion beamlets are also noted.

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**#091 - SUPERINTENSE LASER-DRIVEN ION ACCELERATION WITH NANOSTRUCTURED TARGETS**

Matteo Passoni (I) - Politecnico di Milano

Superintense laser-driven ion acceleration represents today a research topic of unique interest, both for fundamental reasons and for its potential towards future applications [1, 2]. Great efforts are devoted in finding suitable ways to meet specific requirements in terms of ion properties. Further developments in laser technology, which will guarantee laser pulses with unprecedented parameters in the next future, should open the possibility to achieve so far unexplored regimes. However, the development of solutions based on sufficiently robust target concepts to provide, at the same time, a major improvement in the laser-to-ion conversion efficiency, increasing the coupling of the laser pulse with the target, and to relax the technological constraints preventing their use at high repetition rate, is of paramount importance to demonstrate that laser-driven ion acceleration may really become useful in the next future for at least some of the conceived scientific and technological applications.

This talk will provide a concise review of the relevant state of the art and then will focus on an example of novel multi-layered target concept, in which an ultra-low density nanostructured material ("foam") is superimposed on the surface of a thin Al foil [3-5]. In particular, production methods of such targets and recent laser-driven ion acceleration experiments performed at the Ultra-short Quantum Beam Facility of the GIST Institute (South Korea) will be presented and discussed, also thanks to the support of dedicated particle-in-cell numerical simulations. It will be shown that a significant enhancement in the maximum energy of accelerated ions is achieved for foam-attached targets with optimized parameters, with respect to the case of Al foils.

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**#092 - Asymptotic Expansion of the Fluid-Maxwell's equations system in magnetized plasmas**

Alessandro Cardinali (I) - ENEA

The propagation of the electromagnetic modes from low (Radio Waves) to high frequencies (TeraHertz) in a magnetized plasma is described by means of the Maxwell's equation system coupled to the plasma dynamics that can be modeled by a fluid description of the plasma. In some relevant conditions, after linearizing the fluid equations for both plasma species, an asymptotic treatment of the problem can be given in terms WKB [1] expansion of the fields. At the lowest order a non linear first order partial differential equation for the Phase Integral, formally equivalent to the Hamilton-Jacobi equation in classical mechanics, can be obtained and solved in terms of the ray trajectories, while at the next order a transport equation for the slowly varying wave energy density can be obtained and solved, thus allowing to reconstruct the electric field inside the plasma. Examples of solution for the propagation of the Lower Hybrid Waves, relevant in the heating and current drive of laboratory plasmas confined in toroidal devices (tokamak) oriented to the research on thermonuclear fusion, and the propagation of Whistler Radio Signal in the upper ionosphere will be shown and discussed.

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### #093 - Turbulence, transport and structure properties in the simply magnetised toroidal plasma device THORELLO

*Ruggero Barni - Universita' degli Studi di Milano-Bicocca/Dipartimento di Fisica Occhialini*

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Turbulence, transport and structure properties  
in the simply magnetised toroidal plasma device THORELLO

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Experimental investigation of magnetised plasma turbulence is actively pursued in fusion aimed as well as in basic plasma physics toroidal devices. In particular the understanding of turbulent transport mechanisms has a great interest for the improvement of the magnetic confinement. Here we report the results of an experimental investigation of plasma parameters fluctuations of a turbulent, low beta, low temperature plasma with a simply magnetised torus configuration. Experiments have been performed in the Thorello device, operating at the University of Milano-Bicocca. There a low temperature, high density plasma can be produced in a steady configuration for long times in a hydrogen low pressure discharge. Plasma parameters have been studied by means of multiple pin electrostatic probes and fairly long time series of fluctuations have been obtained and correlated.

At the edge of magnetic confinement devices, a large fraction of anomalous particles and energy transport is attributed to the propagation of density blobs [1]. These are isolated and intermittent structures, with density and temperature above the surrounding plasma, extending along field lines and propagating away from the bulk. In this contribution we discuss some properties of plasma structures that develops and propagates in the edge region. In particular we assess the role of transport flux events, defined by the simultaneous enhancement of plasma density and radial ExB velocity. Effects of such events on plasma transport (particle flux) has been analyzed for different scenarios.

Turbulence can be characterized also through the nonlinear interaction between Fourier components, which leads to a nonlinear energy transfer that moves the energy to different spatio-temporal ranges. Multispectral analysis is one of the techniques suitable to investigate the wave-wave couplings. Here we report results concerning the nonlinear spectral transfer function [2]. Evidence of the presence of an inverse energy cascade of the spectral energy is obtained in regions at the edge of the plasma column. These findings are compared with the spatiotemporal evolution of density structures observed in the device.

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### #094 - Time-resolved emission from bright hot pixels of an active region observed in the EUV band with SDO/AIA and multi strand loop modeling

*Edris Tajfirouze - university of palermo*

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Evidence for small amounts of very hot plasma has been found in active regions and might be the indication of an impulsive heating, released at spatial scales that are smaller than the cross section of a single loop. We investigate the heating and substructure of coronal loops by analyzing the light curves in the smallest resolution elements of solar observations in two EUV channels (94-Å and 335-Å) from the Atmospheric Imaging Assembly on-board the Solar Dynamics Observatory. We model the evolution of a bundle of pulse-heated strands by means of a hydrodynamic 0D loop model.

The light curves obtained from the random combination of those of single strands are compared to the observed light curves either in a single pixel or in a row of pixels, simultaneously in the two channels and using two independent methods: one is an artificial intelligent system and the other is a simple cross-correlation technique.

We explore the space of the parameters to constrain the distribution of the heating events, their duration and their spatial size,

and, as a feedback on the data, their signatures on the light curves.

Both comparison methods are unanimous in an individual set of parameter related to a particular set of realizations to reproduce the observed feature of single pixel and a row of pixels. The best agreement is obtained with a relatively shallow distribution of events (power law with index 1.5), that can be expected for a homogeneous region, a short duration of the events (less than 1 min) and a relatively large number of events (1000) inside a pixel. The feedback on the data indicates that bumps in the light curves, especially in the 94-100 channels, are signatures of a heating excess with a delay of a few minutes.

#### #095 - Neutron emission from beam-target reactions studied at the ELISE neutral beam test facility

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Neutron measurements are proposed for the SPIDER and MITICA Neutral Beam Injection (NBI) prototypes in Padua as a means to diagnose the footprint of the deuterium beam when it hits the beam calorimeter. Neutron emission is here due to reactions between the beam and the adsorbed deuterons in the target and thus depends on the deuteron absorption level in the beam calorimeter.

We have investigated such process at the ELISE facility of the Max Planck Institut für Plasmaphysik in Garching. ELISE is a "half size" ITER NBI test facility capable to accelerate negative hydrogen and deuterium ions up to 60 kV and to perform plasma operations of the radio frequency ion source for up to 1 hour.

A first measurement campaign was carried out in 2014 during the initial deuterium operations of ELISE with a liquid scintillator detector installed in vicinity of the dump and that was used as global neutron monitor. The detector had standard neutron/gamma-ray discrimination capabilities and known response function obtained from a dedicated calibration at a neutron generator in Peking University. The collected data showed an increasing neutron rate as a function of time, until a saturation level is reached, and were generally in agreement with calculations based on local mixing model of deuterium deposition in the target up to a concentration of 20% of the copper atoms. Deviations up to 40% from the predicted neutron yield were however observed at the highest beam currents (10 A). These could be either due to neglected spatial profile variations of the beam power deposited on the target or indicate physics mechanism beyond the local mixing model, such as diffusion of deuterium at saturation due to temperature effects.

A new, dedicated experiment is presently ongoing at ELISE to understand neutron emission at the highest beam currents, which are of special relevance to validate calculations for SPIDER/MITICA and, more generally, to predict neutron emission from beam target reactions, such as in compact neutron sources. The experiment makes use of detailed beam diagnostic data from calorimetry and infra-red systems, which can be combined to track changes in the beam power deposition profile on the dump. Preliminary results from the new experiments will be presented and compared with data at low beam currents.

This work was set up in collaboration and financial support of F4E.

#### #096 - A quantitative modeling of the "slingshot" laser-driven acceleration of plasma electrons

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We have recently proposed [1-3] a new laser-driven acceleration mechanism based on the violent impact of an ultra-short and ultra-intense laser pulse against the electrons belonging to a superficial thin layer of a low-density plasma (or gas, provided the pulse is sufficiently intense to locally cause its complete ionization). The interplay among the strong ponderomotive effect, the excited restoring electric field (originated by charge separation) and the finite size of the laser spot causes the expulsion of electrons from the plasma surface with high energy in the direction opposite to that of the pulse propagation ("slingshot effect"). We now reduce [4] the relevant magnetohydrodynamical equations to a pair of first order differential equations (or a collection of) and thus give a reliable quantitative description of the effect for a broad range of intensities and initial densities, both smooth and step-shaped. Its experimental verification seems to be feasible and, if confirmed, would provide a new laser-driven acceleration mechanism for electrons.

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**#097 - Ferroelectric and hybrid magnetic-ferroelectric tunneling junctions based on BaTiO<sub>3</sub> barriers**

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Tunnelling junctions with ferroelectric barriers are currently under investigation for different applications, including ferroelectric memories [1] and memristive devices [2]. Both are based on the large values of the tunnelling electro resistance (TER), i.e. the normalized variation of the tunnelling resistance upon reversal of the ferroelectric polarization, which represents the stored information. Another state variable can be introduced if the electrodes are ferromagnetic, in the so called "hybrid magnetic-ferroelectric tunnelling junctions", where at least four distinct memory states can be found, depending on the configuration of the ferroelectric polarization and electrodes magnetization. [3]

In this paper we present some recent results obtained on tunnelling junctions involving epitaxial BaTiO<sub>3</sub> (BTO) barriers. First we report on TER of Pt/BaTiO<sub>3</sub>/La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> (Pt/BTO/LSMO) purely ferroelectric tunnel junctions. [4] Record values of TER, up to 3 x 10<sup>4</sup> %, have been found at room-temperature on large-area junctions (A = 4 to 900 μm<sup>2</sup>), made using standard lithography techniques. Beyond this, a radically new experimental observation is made. It is found that the capacitance of the junctions is bias-voltage and frequency dependent, due to the modification of the barrier thickness arising from the modulation of a depletion layer existing close to the BTO/LSMO interface.

Then we discuss the case of fully epitaxial Co(6ML)/Fe(2ML)/BTO/LSMO hybrid tunnelling junctions. By XMCD measurements on patterned Co(6ML)/Fe(2ML)/BTO/LSMO micro-capacitors, we found that, at RT, the average magnetization of the FeO<sub>x</sub> interfacial layer disappears for the dielectric polarization vector of BTO pointing outwards from the FeO<sub>x</sub> layer. [5] A "giant" interface inverse magnetoelectric effect results, which has been exploited in micron sized hybrid magnetic-ferroelectric tunneling junctions, based on the same stack used for XMCD. We found an intriguing behavior of the bias dependence of the tunneling magnetoresistance (TMR), which can be explained in terms of symmetry based spin filtering of Fe states through the BTO epitaxial barrier. Furthermore, 100% modulation of the TMR has been found upon reversal of the BTO polarization, with a huge suppression of the TMR for the BTO polarization pointing outwards from the Fe layer, in full agreement with XMCD measurements.

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**#098 - Oxide heterostructures with tunable spin polarization and superconductivity**

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The discovery of an electric field tunable 2DEG at the interface between LaAlO<sub>3</sub> and SrTiO<sub>3</sub> band insulators [1] sparked an enormous interest in condensed matter community, also due to the growing demand for new functional materials for electronic applications. While some properties of this 2DEG are well established (tunable superconductivity and spin orbit coupling, for instance) others are still debated. Magnetic effects have been reported by some groups but their origin, if intrinsic or extrinsic, is controversial.

We engineered an oxide heterostructure inserting two unit cells of ETO between SrTiO<sub>3</sub> and LaAlO<sub>3</sub> (LAO/ETO/STO)[2]. ETO acts as δ-doping material, resulting in a spin-polarized 2D electron system. We present a detailed characterization of the LAO/ETO/STO 2DEG, performed using polarization dependent x-ray absorption spectroscopy, to study the orbital reconstruction and the spin-splitting of titanium 3d-states; and magneto-transport measurements, giving evidence of spin-orbit coupling, of an itinerant ferromagnetism, and of a Kondo-like behavior in the underdoped region. Finally, ultra low temperature measurements show a superconducting transition. All these properties are tunable using field effect.

The results are condensed in a rich phase diagram, showing how LAO/ETO/STO spans different ground states as function of the carrier density.

The interplay among magnetic exchange interactions, superconductivity and spin-orbit coupling could make the LAO/ETO/STO system an extraordinary platform to realize topologically non-trivial edge states at the interface between transition metal oxides [3].

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**#099 - Electronic and magnetic properties of quantum materials as seen by X-ray electron spectroscopies.**

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The collective behaviour of matter is one of the central topics of modern science and technology. Collective quantum phenomena in materials arise from the interplay between quantum mechanics and interactions in many-particle systems — i.e., materials for which the interactions between particles cannot be treated in a semi-classical manner. Recent advances in material growth and structural optimization processes, combined with improved analytical methods, led to the ability of understanding, designing, and controlling systems with tailored electronic and magnetic properties. In the wealth of topics linked to quantum materials, dimensionality (1D and 2D) effects play a fundamental role: new collective phenomena, e.g. quantum size confinement, orbitally/magnetically driven interface effects, topological properties have been recently observed in 'less than 3D' materials.

The chemical sensitivity, the variable polarization and the tunable depth information of X-ray based techniques are valuable analytical tools to study the quantum nature of matter and in particular to reveal new electronic and magnetic properties. In this talk, selected examples focused on complex correlated oxides and their interfaces, diluted magnetic systems, ferromagnetic topological insulators and transition metal dichalcogenides will be presented [1-3], where magnetic coupling via proximity effects and novel, depth dependent, electron screening behavior will be discussed.

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**#100 - GeTe: a novel paradigm for spintronics with Ferroelectric Rashba Semiconductors**

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Semiconductor spintronics has for long concentrated on devices, such as the Datta-Das spin-FET, where the semiconductor plays a passive role. In the compelling quest for multifunctionality and non-volatility, however, a breakthrough would come from turning the semiconductor into an active element. We recently proposed to radically change the perspective of current semiconductor spintronics by bringing in a novel functionality, i.e. the coupling between ferroelectricity and Rashba effects in Ferroelectric Rashba Semiconductors (FERSC). The test-case material is represented by GeTe, for which theory predicts a giant Rashba spin-splitting reversible by switching of the ferroelectric polarization [1]. To exploit this peculiar property, different architectures of spin transistors can be proposed. For instance a spin-FET, whose impedance can be electrically controlled thanks to the interplay between Rashba effects, electronic spin precession and ferroelectricity. Noteworthy, non-volatility is ensured by the permanent polarization of the GeTe channel, so that a new generation of spintronics devices integrating memory and computing functions can be envisaged.

In this paper we provide evidence for the FERSC properties of GeTe via piezo force microscopy (PFM) and Spin and Angular Resolved PhotoEmission Spectroscopy (SARPES). In GeTe(111) thin films [2] with outwards remanent ferroelectric polarization, a huge Rashba splitting of the valence band has been measured at low temperature. The band dispersion and the sense of circulation of spins is in agreement with that expected from DFT calculations for an outwards dielectric polarization [3]. This demonstrates the intimate link between ferroelectricity and Rashba, which is the basis for the exploitation of FERSC. Preliminary experiments of spin pumping on Fe/GeTe heterostructures display the existence of an inverse Spin Hall effect, which is consistent with the Rashba bands detected by ARPES.

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**#101 - Topological skyrmion dynamics in perpendicular magnetic materials excited by a spin-polarized current**

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Topological and non-topological magnetic solitons can exist either as static (vortices, bubbles, skyrmions, etc.) or dynamical (droplets, vortex-antivortex pair, etc.) states (limit cycles) in both conservative and dissipative magnetic systems. In this work it is

shown the effect of the interfacial Dzyaloshinskii–Moriya Interaction ( $i$ -DMI) [1] on the topology of droplets excited by a localized perpendicular spin-polarized current. According to micromagnetic simulations it is shown that the phase diagram  $i$ -DMI as a function of the polarized current at zero magnetic field exhibits a complex scenario with regions characterized by static and dynamic states. In the dynamical part, it is possible to identify topological stable and unstable regions. The topological stable regions are linked to the excitation of droplets with skyrmion number either equal to one (topological) or zero (non-topological). The zero skyrmion number droplets are characterized by the non-stationary time domain excitation of both topological and non-topological droplets modes. The transition between these two modes is coupled to an emission of incoherent spin-waves. It is also developed an analytical model demonstrating that the topological droplet can be seen as a linear radial mode of a static skyrmion state stabilized by a perpendicular spin-polarized current. The analytical frequency of the topological droplet mode is expressed as the solution of an algebraic equation written in terms of the magnetic parameters. The results obtained by means of the analytical model confirm the red-shift behaviour of the topological mode frequencies as a function of the current density predicted by micromagnetic simulations. The interplay between topology and dynamics is discussed by introducing the notion of topological degeneracy according to which two topological droplet textures (hedgehog-like and vortex-like, respectively) having different ground-state energies are characterized by the same topological charge. The analysis of the symmetry properties of the linearized equations of motion demonstrates the non-reciprocal role of the spin polarized current on the topological mode dynamics [2].

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### #102 - Solitons on Heisenberg spin chains and qubit manipulation

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One of the difficulties commonly met when solid-state realizations of quantum computers are proposed, is that of addressing and manipulating the single qubits of a quantum register without affecting the neighbouring ones. We here describe the proposal of using magnetic solitons propagating along spin chains as a suitable mean for qubit manipulation. Indeed, the robustness of the propagation of such nonlinear excitations against perturbations, like thermal noise, makes them natural candidates for the faithful transmission of signals between distant parties. Solitons are known analytical solutions of the equations of motion of classical spin chains on continuous support, and the experimental data show clear signatures of the solitonic contributions to the thermal properties of quasi one-dimensional magnetic materials.

In view of the possible use of solitons for qubit manipulation, we present a practical scheme to achieve the generation of soliton-like excitations on discrete classical Heisenberg chains by applying a time-dependent magnetic field to one end of the chain. We present a numerical investigation of the resulting dynamics of the discrete chain, showing the effective injection of solitons under the proposed scheme and their robustness against thermal disorder. Finally, we propose a setup where the generated soliton represents a magnetic signal travelling along the chain which eventually reaches a distant qubit, realized by a spin 1/2 magnetic moment coupled to the chain, in order to manipulate its quantum state. Numerical results confirm that solitons are indeed suitable for this task, giving the possibility to remotely control the qubit state by an appropriate choice of soliton shape and qubit-chain coupling parameters.

### #103 - Anomalous magnetization of a carbon nanotube as an excitonic insulator

*Massimo Rontani - CNR-NANO Research Center S3*

We suggest that an undoped carbon nanotube might be an excitonic insulator---the long-sought phase of matter that was proposed by Keldysh, Kohn, and others fifty years ago as a paradigm of strongly correlated insulator alternative to the Mott-Hubbard picture. We show theoretically that the Bose-Einstein condensation of triplet excitons, driven by intervalley exchange interaction, spontaneously occurs at thermodynamic equilibrium if the tube radius is sufficiently small [1]. Our claim contradicts previous studies that neglected the coupling between K and K' valleys [2]. We predict that the signatures of exciton condensation are its sizable contributions to (i) the energy gap, (ii) the spin-orbit interaction, and (iii) the magnetic moment per electron. The increase of

the gap might have already been measured, albeit attributed to the Mott insulating state [3], whereas giant values of spin-orbit energy splittings were recently reported with no explanation [4]. The enhancement of the quasiparticle magnetic moment is a pair-breaking effect that counteracts the weak paramagnetism of the ground-state condensate of excitons. This property could rationalize the anomalous magnitude of magnetic moments recently observed in different ultraclean devices close to charge neutrality [5].

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**#104 - Magnetism in Fe-based Superconductors - The Various Ways to Coexist***Hubertus Luetkens (I) - Paul Scherrer Institute*

Magnetism and superconductivity are key elements in the electronic phase diagram of all unconventional superconductors, such as the high- $T_c$  cuprates, heavy-fermion, organic and Fe-based superconductors. Muon spin rotation ( $\mu$ SR) is a powerful tool for studying the exact nature of the transition from the antiferromagnetic to the superconducting phase in high- $T_c$  superconductors as a function of a control parameter such as doping or pressure. In this context, it is of special advantage that  $\mu$ SR, as a local probe, is sensitive to both the superconducting and magnetic volume fractions and to the respective order parameters, that fundamental microscopic parameters such as the magnetic penetration depth can be determined absolutely, and that  $\mu$ SR is extremely sensitive to small-moment and short-range magnetic order.

From the very beginning of research on Fe-based superconductors in 2008,  $\mu$ SR has contributed important information. It is widely recognized as one of the key techniques for investigating fundamental magnetic and superconducting properties, as well as testing for microscopic competition or coexistence of the magnetic and superconducting ground states.

Interestingly, in the electronic phase diagrams of Fe-based superconductors we find various ways of how the magnetic and superconducting order can coexist, namely in i) an electronically and structurally phase separated way, ii) with a competition about the volume, iii) with a competition about the magnetic moment, iv) a coexistence without competition, v) with magnetism as a necessary prerequisite for superconductivity and vi) with no coexistence at all.

In this talk, after a short introduction to  $\mu$ SR, we will review our  $\mu$ SR results on the magnetic and superconducting properties of various families of Fe-based superconductors.

**#105 - Thermoelectric properties of iron-based superconductors***Marina Putti (I) - University of Genova and CNR-SPIN*

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Iron-based materials in the last years have been a gym for solid state physicists and material scientists, showing unexpected properties both in the antiferromagnetic and in the superconducting state.

In this talk, we review thermoelectric transport properties of iron-based superconductors and parent compounds. We discuss possible physical mechanisms into play in determining the Seebeck effect, from whence one can extract information about Fermi surface reconstruction, multiband character, coupling of charge carriers with spin excitations and its relevance in the unconventional superconducting pairing mechanism. Additional information is obtained from the analysis of the Nernst effect, whose enhancement in parent compounds must be related partially to multiband transport and low Fermi level, but mainly to the presence of Dirac cone bands at the Fermi level. A comparison between the phenomenology of thermoelectric behavior of different families of iron-based superconductors and parent compounds allows to evidence the key differences and analogies, thus providing clues on the rich and complex physics of these fascinating unconventional superconductors.

**#106 - Electronic Structure and High Temperature Superconductivity in FeSe/SrTiO<sub>3</sub> Films and Related Iron-Based Superconductors***Xingjiang Zhou (I) - Institute of Physics, Chinese Academy of Sciences*

In this talk, I will report our recent angle-resolved photoemission (ARPES) work on the electronic structure and superconductivity of FeSe/SrTiO<sub>3</sub> thin films: [1]. Unique electronic structure and superconducting gap in single-layer FeSe/SrTiO<sub>3</sub> film; [2]. Phase diagram and observation of superconductivity at 65K in single-layer FeSe/SrTiO<sub>3</sub> film; [3]. Dichotomy of electronic structure and superconductivity between the single- and double-layer FeSe/SrTiO<sub>3</sub> films; [4]. Insulator-superconductor transition in single-layer FeSe/SrTiO<sub>3</sub> films. I will also report our latest work on the new FeSe-based superconductor, (Li,Fe)OHFeSe, that shows strikingly similar electronic structure as the superconducting single-layer FeSe/SrTiO<sub>3</sub> films[5]. Implications of these observations on the superconductivity mechanism of the iron-based superconductors will be discussed.

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**#107 - Ru-doping on Fe-based superconductors: structural versus electronic effects***Alessandra Continenza - Università degli studi dell'Aquila*

*Other Authors: Michele Retliccioli (Università degli studi dell'Aquila e University of Vienna), Cesare Franchini (University of Vienna), Gianni Profeta (Università degli studi dell'Aquila)*

Since their discovery in 2008, the Fe-based pnictides constitute a widely studied class of materials, showing superconducting behavior upon doping or applied pressure. However, the mechanism driving transition to the superconducting state is not clear as there are still many different issues that need careful investigation. One of these, concerns isovalent transition metal substitutions and their different effects on different classes of materials. This is the case, for example, of Ru-doping on the transition metal sites of the Fe-As layers in BaFe<sub>2</sub>As<sub>2</sub> (Ba-122) and LaOFeAs (La-1111). Although Ru is considered to be isovalent with Fe, it is seen to induce superconductivity in Ba-122 up to rather large Ru-concentrations (35%), while it is seen not to affect the La-1111 compound and even suppress superconductivity in F-doped LaOFeAs (La-1111) samples making the transition temperature linearly decrease. Thus, the question arises: why does Ru-doping show such different behavior on 122 and 1111 systems? In order to answer to this question, by means of first principles calculations we perform conceptual simulated experiments to i) separate out pure-electronic from pure-structural contributions to the states at the Fermi level and ii) to compare step by step the two compounds.

### #108 - Enhancement of low-frequency fluctuations and superconductivity breakdown in Mn-doped La<sub>1-y</sub>Y<sub>y</sub>Fe<sub>1-x</sub>Mn<sub>x</sub>AsO<sub>0.89</sub>F<sub>0.11</sub> superconductors

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The introduction of impurities in superconducting materials is a powerful method to unravel some of their intrinsic microscopic properties. In this study we focus on the peculiar case of Mn impurities substitution on the Fe site in optimally doped La<sub>y</sub>Y<sub>y</sub>FeAsO<sub>0.89</sub>F<sub>0.11</sub> ( $y = 0$ ;  $y = 0.2$ ). In the  $y = 0$  series a very low critical concentration of Mn ( $x = 0.2\%$ ) is enough to destroy the superconducting phase and to induce a quantum phase transition to a magnetic state [1]. On the other hand, in the  $y = 0.2$  series the chemical pressure induced by La for Y substitution stabilizes superconductivity, which is observed to vanish only for Mn contents an order of magnitude larger than for  $y=0$  [2]. For both series a peak in the <sup>19</sup>F NMR nuclear spin-lattice relaxation rate  $1/T_1$  emerges upon Mn doping and gets significantly enhanced on approaching the quantum phase transition between the superconducting and magnetic phases. The magnetic field dependence of  $1/T_1$  indicates slowing down of the frequency of the fluctuations to the MHz range occurs. <sup>19</sup>F NMR linewidth measurements show that for similar Mn contents magnetic correlations are more pronounced in the  $y = 0$  series, at variance with what one would expect for stripe spin correlations. These observations suggest that Mn doping tends to reduce fluctuations at  $Q = (\pi/a, 0)$  and to enhance other low-frequency modes. These experimental results are discussed in the framework of spin-glass like fluctuations developing in Néel correlated regions around the Mn impurities as well as considering the role of nematic fluctuations.

[1] F. Hammerath et al. Phys. Rev. B 89 (2014) 134503

[2] F. Hammerath, M. Moroni et al. arXiv:1504.04352

### #109 - Mutual independence of T<sub>c</sub> and superfluid density under pressure in optimally-doped LaFeAsO<sub>1-x</sub>F<sub>x</sub>

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The superconducting properties of LaFeAsO<sub>1-x</sub>F<sub>x</sub> in conditions of optimal electron-doping are investigated upon the application of external pressure up to  $P = 23$  kbar [1]. Measurements of muon-spin spectroscopy and dc magnetometry evidence a clear mutual independence between the critical temperature  $T_c$  and the low-temperature saturation value for the ratio  $n_s/m^*$  (superfluid density over effective band mass of Cooper pairs). Remarkably, a dramatic increase of 30 % is reported for  $n_s/m^*$  at the maximum pressure value while  $T_c$  is substantially unaffected in the whole accessed experimental window. Such a dramatic increase under  $P$  while keeping  $T_c$  constant is an unprecedented observation for any superconducting material, to the best of our knowledge. We provide

evidence from density-functional theory (DFT) calculations that this result should not be associated to an induced change in the fermiology of  $\text{LaFeAsO}_{1-x}\text{F}_x$  or, equivalently, to a  $P$  dependence of  $m^*$ . We argue and demonstrate that the explanation for the observed results must take the effect of non-magnetic impurities on multi-band superconductivity into account. In particular, the unique possibility to modify the ratio between intra-band and inter-bands scattering rates by acting on structural parameters while keeping the amount of chemical disorder constant is a striking result of our proposed model.

[1] G. Prando *et al.*, arXiv:1502.02713 (2015)

#### #110 - LOW TEMPERATURE- HIGH FIELD PERFORMANCES OF IRON CALCHOGENIDES THIN FILMS

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Among the various families of Fe-based superconductors, iron chalcogenides, while present a transition temperature not particularly high, show great advantages for potential applications in high field, albeit at liquid helium temperature. In thin films, the strain can push the critical temperature up to 21K, the critical field up to more than 50 T and the irreversibility field close to this value. The critical current and its anisotropy heavily depend on the type of substrate used for the deposition. It is possible to reach values up to 1 MA/cm<sup>2</sup> at liquid helium temperatures and self-field with weak magnetic field dependence and without appreciable anisotropy. In this study, we will show what are the defects acting as pinning centers for different substrates and how the shape of the pinning centers determines the anisotropic observed currents. Finally, in the case of STO, we present the first measurements on FeSeTe thin films deposited on bi-crystals showing that, differently from HTS, the high angle grain boundary is less limiting the supercurrent. Experiments indicate that the current is not appreciably depressed up to a misorientation angle of 10 degrees.

**#111 - Giant Oscillating Thermopower at Oxide Interfaces***Daniele Marré (I) - University of Genova and CNR-SPIN*

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Understanding the nature of charge carriers at the  $\text{LaAlO}_3/\text{SrTiO}_3$  interface is one of the major open issues in the route towards the full comprehension of the charge confinement phenomenon in oxide heterostructures. Thermoelectric spectroscopy is a formidable tool for the exploration of the electronic properties of doped semiconductors, since its signal is closely related to the density of states around the Fermi energy.

In this work, we explore thermopower in  $\text{LaAlO}_3/\text{SrTiO}_3$  at low temperature as a function of gate field, in order to monitor the electronic properties at varying doping concentration. In particular, under large negative gate voltage, corresponding to the strongly depleted charge density regime, thermopower displays record-high negative values of the order of  $10^4$ - $10^5$  mV/K, oscillating at regular intervals as a function of the gate voltage. The huge thermopower magnitude can be attributed to the phonon-drag contribution, while the oscillations map the progressive depletion and the Fermi level descent across a dense array of localized states lying at the bottom of the Ti 3d conduction band. This study is the first direct evidence of a localized Anderson tail in the two-dimensional (2D) electron liquid at the  $\text{LaAlO}_3/\text{SrTiO}_3$  interface.

**#112 - Non-perturbative effects of electron-phonon interaction in strongly disordered system***Sergio Ciuchi - University of L'Aquila*

*Other Authors: Domenico Di Sante (Dipartimento di Scienze Fisiche e Chimiche Università dell'Aquila, Italy), Simone Fratini (Insitut Nééel, CNRS Grenoble, France)*

Using a combinations of DMFT, Typical Medium Theory, and Self-Consistent Non Crossing Approximation we study the half-filled disordered Holstein model. We found that the electron-phonon interaction acts synergistically with disorder to drive the states near the Fermi energy toward localization. The resulting insulating state changes continuously its character passing from a polaronic insulator at weak disorder to an Anderson insulator at weak electron-phonon coupling. In the metallic phase polaronic signatures could be found up to very small values of electron-phonon coupling. Phonon quantum fluctuations instead favor metallic phase at zero temperature but well into the insulating phase they contribute to increase the resistivity.

## References

D. Di Sante, S. Ciuchi

"Strong interplay between electron-phonon interaction and disorder in low doped systems."

[Phys. Rev. B 90, 075111 \(2014\)](#)**#113 - Using magnetic stripes to stabilize superfluidity in electron-hole double monolayer graphene***Luca Dell'Anna - Dipartimento di Fisica e Astronomia "G. Galilei", Università di Padova*

Experiments have confirmed that double monolayer graphene cannot generate finite temperature electron-hole superfluidity. This has been shown to be due to very strong screening of the electron-hole pairing attraction. The linear dispersing energy bands in monolayer graphene prevent attempts to reduce the strength of the screening. We propose a new hybrid device in which the two sheets of monolayer graphene are placed in a modulated periodic perpendicular magnetic field. Such a magnetic field preserves the isotropic Dirac cones of the original monolayers but it reduces the slope of the cones so that the monolayer Fermi velocity  $v_F$  is smaller. We show that with current experimental techniques, this reduction in  $v_F$  can sufficiently weaken the screening to permit electron-hole superfluidity at measurable temperatures.

**#114 - Atomic scale view of the early stages of a metal oxidation: Scanning Tunneling Microscopy and Spectroscopy study of the oxidation of Co ultrathin films***Andrea Picone - Politecnico di Milano*

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Oxidation of metallic surfaces plays a fundamental role in many fields of modern nanotechnology, spanning from heterogeneous (nano) catalysis [1], corrosion protection [2], and metal/oxide layered structures [3,4]. From a more fundamental point of view, a detailed understanding of the atomistic mechanisms driving the transition from the metallic to the oxide phase is far from being conclusively achieved. Does the oxide nucleation occur over the atomically flat terraces or starts from surface defects sites? Which is the evolution of the surface electronic structure during the early stages of oxygen exposure? If compared to other surface science spatial averaging techniques, the number of Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) studies investigating the early stages of metals oxidation is still scarce. Indeed, the oxidation process often induces the development of rough surfaces or even amorphous structures, rendering their investigation by means of STM a challenging task. In this contribution it will be shown that the oxidation of nanometer-thick Co films deposited on Fe(001) can be followed step by step, from the early stages of subsurface oxygen penetration, until a closed oxide overlayer is fully developed. Highly resolved STM images allow to resolve the atomic details of the oxide wetting layer, while STS and constant current topographic images acquired at variable tunneling conditions reveal the band gap opening since the early stages of oxide nucleation.

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### #115 - A method of surface texturization of silicon by a maskless plasma process

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Deep surface texturization boosts novel applications of Silicon and improves its performances in selected fields. Micrometric or sub-micrometric texturized Silicon, increases optical absorption, what may contribute to improve optical detection and solar cell efficiency [1,2]. The definition of pillars and grooves also functionalizes the surface as a scaffold for biomedical applications, by inducing selective antibacterial characteristics [3]. In this work we introduce a reactive mask-less method to achieve deep texturing of Silicon by using  $\text{CF}_4/\text{H}_2$ -based processing in a Plasma Enhanced Chemical Vapour Deposition (PECVD) system [4]. The RF (13.56 MHz) powered electrode of the PECVD apparatus works as a support for the substrates. Operating parameters in the range of 0.05-0.1 mbar (gas pressure), 200-280 W (RF power) and 20-30 min (processing time) issue random pillars as high as 300 nm, with diameters in the range of 100-150 nm. The plasma has been investigated in the different operating conditions by optical emission spectroscopy (OES). OES spectra show the presence of F, C, H neutral atomic lines and  $\text{CF}_2$  ro-vibronic narrow bands ( $\tilde{A}^1B_1 - X^1A_1$ ) in the 245-325 nm range; also CO and  $\text{CO}^+$  ro-vibronic bands due to the oxygen desorbed by the chamber walls are identified. As confirmed from OES, the plasma process takes place in high fragmentation regime and so many radicals are produced, in particular, the main precursors for the deposition ( $\text{CF}_x$ ) and etching ( $\text{F}^*$ ) are evident.

In order to understand which reactions are at the basis of the mask-less etching process and to assess the nature of the passivation layer on the surface and in the bulk of the Si samples, OES analysis has been combined with results from XPS, SIMS and Scanning Auger Micro-spectroscopy.

Reflectance of the treated silicon surface has been characterized by UV-Vis spectrophotometer equipped with an integrating sphere. An overall average reflectance lower than 10% in the visible and near-IR spectrum has been demonstrated.

Mask-less Fluorine plasma-etched black silicon is therefore appealing to increase optical absorption in the solar spectrum. Biomedical applications are under test

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### #116 - Molecular Ordering at the Interface Between Liquid Water and Rutile $\text{TiO}_2(110)$

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The pivotal importance of TiO<sub>2</sub> as a technological material involves most applications in an aqueous environment, but the single-crystal TiO<sub>2</sub>/bulk-water interfaces are almost completely unexplored, since up to date solid/liquid interfaces are more difficult to access than surfaces in Ultra High Vacuum (UHV). Only a few techniques (as Scanning Probe Microscopy) offer the opportunity to explore these systems under realistic conditions. We have studied the rutile TiO<sub>2</sub>(110) surface immersed in high-purity water by in-situ scanning tunneling microscopy (STM). The large-scale surface morphology as obtained after preparation under UHV conditions remains unchanged upon prolonged exposure to bulk water. Moreover, in contrast to UHV, atomically resolved images show a two-fold periodicity along the [001] direction, indicative of an ordered structure resulting from the hydration layer. This is consistent with density-functional theory based molecular dynamics (DFT-MD) simulations where neighboring interfacial molecules of the first water layer in contact with the bulk liquid form dimers. By contrast, this dimerization is not observed for a single adsorbed water monolayer, i.e. in the absence of bulk water.

### #117 - Synthesis and photocatalytic properties of hydrogenated TiO<sub>2</sub> nanoplumes

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In the last years, the synthesis of a wide range of advanced inorganic materials (nanocomposite thin films, patterned surfaces and nanostructures) was extensively studied. In particular, the semiconducting oxide TiO<sub>2</sub> has attracted remarkable interest, for its outstanding applications: from solar cells to self-cleaning and water purification.

In this work, we investigate the photoactive properties of TiO<sub>2</sub> nanoplumes. The original material was synthesized by a simple chemical etch, in peroxide solution, of a Ti film deposited by sputtering. The system was morphologically and structurally characterized by scanning and transmission electron microscopy, x-ray diffraction. The band gap of nanoplumes was evaluated by optical transmittance and reflectance measurements, and compared by annealed nanoplumes and standard TiO<sub>2</sub> film. Nanoplumes shows a lower band-gap energy than TiO<sub>2</sub> film, with an energy gap of 2.0 eV against 3.2 eV, making the material sensitive to visible light. The synthesized materials revealed a remarkable efficiency in the photo-degradation of methyl blue in water not only under UV light, but also under VIS light irradiation. In particular, the nanoplumes exhibited a photo-degradation reaction rate that is ~ 5 times the rate of the TiO<sub>2</sub> flat film in the UV and ~ 6 times in the VIS. The photocatalytic activity has been correlated to the physical-chemical structures of the sample. The antibacterial activity was tested by CFU count using *Escherichia coli* as a model organism. It is a well-known Gram-negative bacterium, representative of coliforms and it is considered to be an indicator of fecal contamination in drinking water. In particular, after one hour of exposure under VIS light, bacterial survival dropped down to 17% for the nanoplumes, compared with 72% for the TiO<sub>2</sub> reference sample. The obtained results demonstrate that the originally-synthesized TiO<sub>2</sub> nanoplumes is a promising photoactive material.

### #118 - HIGH TEMPERATURE FUEL CELL ELECTRODES: NEW COMPOSITIONS, MICROSTRUCTURES AND SYSTEMS FOR EFFICIENT UTILISATION OF RENEWABLE FUELS

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Fuel cells will undoubtedly find widespread use in this new millennium in the conversion of chemical to electrical energy, as they offer very high efficiencies and have unique scalability in electricity generation applications. The solid oxide fuel cell (SOFC) offers certain advantages over lower temperature fuel cells, notably its ability to utilise CO as a fuel rather than being poisoned and the availability of high-grade exhaust heat for combined heat and power or combined cycle gas turbine applications. Although cost is clearly a key barrier to widespread SOFC implementation, perhaps the most important technical barriers currently being addressed relate to the electrodes, particularly the fuel electrode or anode. In terms of mitigating global warming, the ability of the SOFC to utilise commonly available fuels at high efficiency, promises an effective and early reduction in carbon dioxide emissions and hence is one of the lead new technologies to improve the environment. In the longer term the ability to utilise waste derived fuels such as biogas will be of critical importance.

Here we describe a series of strategies involving modification of defect chemistry and composition to enhance the electrocatalytic performance of novel perovskite anode and cathode materials that have proved highly successful in reducing polarization resistance and improving output voltage. Results will be presented addressing the use of natural gas, liquid hydrocarbon and carbon-based fuels. Strategies to improve sulphur tolerance, coking resistance and redox stability will be described and the long term prospects discussed. We also report on the microstructural evolution of Mn-containing perovskites impregnated into yttria stabilised zirconia scaffolds on heating and redox cycling. This seems to offer a very attractive structure with extensive triple phase boundary regions being formed where electrochemical reactions can occur.

### #119 - What can we learn from the modeling of elementary steps in energy devices? PEMFC as examples

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Although most of the technologies underpinning renewable energies are (in principle) ready for large-scale implementation, they still require improvement in order to be competitive at both efficiency and economical level with more traditional sources. Design, synthesis, characterization and application of new materials represent a long process often involving several experimental steps each of them requiring significant human and financial resources. Computational materials science can support and speed up this process. Indeed the understanding of microscopic chemical processes at the base of the energy production can provide valuable insights for their improvement. This philosophy will be illustrated with selected examples concerning fuel cells. In particular, it will be illustrated how quantum (DFT) and classical (MD) simulations can give valuable insights on the charge transport mechanism in membranes for fuel cell applications.

### #120 - Infiltrated La<sub>0.8</sub>Sr<sub>0.2</sub>Ga<sub>0.8</sub>Mg<sub>0.2</sub>O<sub>3-d</sub> based cells powered by biogas

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La<sub>0.8</sub>Sr<sub>0.2</sub>Ga<sub>0.8</sub>Mg<sub>0.2</sub>O<sub>3-d</sub> (LSGM) based porous/dense structures were optimized for infiltration of different metal catalysts. Porous anodic substrates with an open porosity larger than 65% were fabricated by using LSGM commercial powders with two different types of porogens: micrometric carbon and polymethylmetacrylate (PMMA). The anodes were pre-sintered at 1250°C for 2 hours to get enough mechanical strength to be used as substrates for spin-coating deposition of micrometric layers of electrolyte. La<sub>0.8</sub>Sr<sub>0.2</sub>Fe<sub>0.8</sub>Co<sub>0.2</sub>O<sub>3-d</sub> was used as cathode and deposited by using a screen-printing oil and firing at 900°C. A 4 M solution of metal (Ni, Co, Cu and their 1:1 mixtures) salts was used for infiltration, dried and heated at 400°C for 30 minutes. Multiple infiltrations were necessary to get a metal catalyst amount of 25wt% that is the required value to get performing electrocatalytic performance. The reduction behavior of impregnated LSGM powders with the same amount of metal catalyst infiltrated in the scaffolds was examined by H<sub>2</sub>-TPR techniques. Ex-situ catalyst activity measurement was used for the initial catalyst screening. The catalytic activity for CH<sub>4</sub> and CO<sub>2</sub> conversion followed the order Ni~Ni-Co>Co>Ni-Cu >>Co-Cu. Co is known to decrease the carbon deposition by different effects such as decreasing the particle size of metallic alloy and thanks to its low affinity toward carbon, the main drawback is the low catalytic activity in comparison with Ni. However, the addition of Co to Ni slightly decreased the catalytic activity, thus Ni-Co alloys may couple the high activity of Ni with the high carbon and sintering resistance of Co yielding higher performing catalysts. The electrochemical measurements were performed on infiltrated cells with the same amount of Ni and Ni-Co in the temperature range between 650 and 750°C. Measurements were performed both in H<sub>2</sub> and CH<sub>4</sub> and results compared. Similar and regarding performance were obtained both for Ni and Ni-Co based cell confirming the results of the catalytic investigation on the corresponding infiltrated LSGM powders. From the electrochemical impedance measurements, both ohmic and polarization resistances of Ni and Ni-Co infiltrated cells slightly increased with time, thus a further investigation on the cell stability is in progress.

**#121 - Some remarks on the development of fuel flexible anodes for Solid Oxide Fuel Cells***Massimiliano Lo Faro - CNR-ITAE**Other Authors: Stefano Trocino (CNR-ITAE) Sabrina Campagna Zignani (CNR-ITAE) Antonino Salvatore Aricò (CNR-ITAE)*

The major energy demand is presently fulfilled by conventional energy resources like petroleum, natural gas, and coal. Petroleum-based fuels are characterized by limited reserves concentrated in certain regions of the world. Thus, the most feasible way to meet the growing demand of energy is to utilize alternative fuels that can be obtained from renewable sources including those derived from biomasses. One of the main implications is consumer's ability to use an increasingly diverse selection of energy sources. New business models could be especially important in the stationary power sector as fuel cell based distributed energy systems become an alternative to or backup for centrally generated power. The European strategy in Energy Systems will improve the efficiency of traditional energy systems and will spread the diffusion of new sustainable energy technologies, and will have therefore an important impact on: European economy; improvement of European companies' competitiveness in high-tech global markets, dependency of the EU from external supply of oil and energy. Small fuel cells systems, typically less than 10kW, are under consideration for many applications that traditional electric utilities have not supplied widely. In this area, solid oxide fuel cells (SOFCs) may enable new companies to enter the power-generation business as equipment providers or heat and electricity providers. The CNR-ITAE has a long and proven experience in SOFCs having contributed to the penetration of this technology into Europe since the early 1980's. In this communication will be reported the CNR-ITAE experience in the electrochemical screening of SOFC anodes under practical operating conditions especially in terms of improved range of fuel use.

**#122 - One pot synthesis of B-site Pd and Ni promoted La<sub>0.6</sub>Sr<sub>0.4</sub>Co<sub>0.2</sub>Fe<sub>0.8</sub>O<sub>3-δ</sub> perovskites: structure-properties relationship***Leonarda Francesca Liotta - Istituto per lo Studio dei Materiali Nanostrutturati (ISMN)-CNR**Other Authors: F. Puleo<sup>1</sup>, A. Longo<sup>1,2</sup>, A. Martorana<sup>3</sup>, V. La Parola<sup>1</sup>, S. Guo<sup>1,4</sup>, C. Lo Cascio<sup>1</sup>, L.F. Liotta<sup>1</sup>. <sup>1</sup>Istituto per lo Studio di Materiali Nanostrutturati (ISMN)-CNR, Via Ugo La Malfa 153, 90146 Palermo, Italy <sup>2</sup>Dutch-Belgian Beamline (DUBBLE), European Synchrotron Radiation Facility (ESRF), B.P. 220, F-38043 Grenoble, France. <sup>3</sup>Dipartimento di Fisica e Chimica, edificio 17, viale delle Scienze, I-90128 Palermo, Italy <sup>4</sup>Northwestern Polytechnical University, Xi'an 710072 PR China.*

An understanding of the structure and dynamics of catalysts during exposure to gaseous reactants is of paramount importance in predicting their performances. In oxidation reactions catalysed by metal oxides, surface coordinatively unsaturated metal cations and oxygen vacancies are the active sites for hydrocarbons and oxygen activation [1]. Even for oxidation reactions catalysed by noble metals supported on reducible oxides, the role of the support in the activation of oxygen is fundamental [2]. On the other hand, it is widely accepted that the rate-limiting steps of O<sub>2</sub> reduction process, occurring at the porous cathode of solid oxide fuel cells, are firstly the surface chemical exchange and then the solid state diffusion of oxygen anions through the oxygen vacancies of the cathode lattice. It appears, therefore, that the synthesis and investigations of metal oxides with tailored oxygen defects are key steps in designing new materials for catalytic and electrochemical applications. LSCF oxides with metal substitution in B-site prepared by different methods, such as solid-state reaction or by impregnation of the perovskite with the metal dopant precursor, have been extensively investigated as new cathodes [3,4]. In the present work, the preparation by one pot citrate method of perovskites with composition La<sub>0.6</sub>Sr<sub>0.4</sub>Co<sub>1-x</sub>Fe<sub>x</sub>O<sub>3-δ</sub> (x=0.2/0.8; M=Pd/Ni) is reported. Characterizations by several techniques (such as XRD, EXAFS, TPR, XPS, TGA, EIS) have been carried out aiming to investigate the effect of the metal (Pd, Ni) insertion on the perovskite structure and oxygen defects. Addition of Pd and Ni to La<sub>0.6</sub>Sr<sub>0.4</sub>Co<sub>0.2</sub>Fe<sub>0.8</sub>O<sub>3-δ</sub> was found to be effective in improving the redox and electrochemical properties. Moreover, preliminary results suggest an increase of oxygen vacancies for Pd and Ni doped oxides, confirming recent data by theoretical DFT calculations used as complementary approach [5]. Acknowledgements The China Scholarship Council is acknowledged for supporting Guo's scholarship in Italy for 2 years. C. Lo Cascio thanks the Regione Siciliana, Progetto N. 20 (ID 11) "Nanomateriali e Nanotecnologie per lo Sviluppo Sostenibile ed il Patrimonio Culturale". References [1] L.F. Liotta, H. Wu, G. Pantaleo, A.M. Venezia, Catal. Sci.&Tech. 3, 3085 (2013). [2] C.A. Mueller, M. Maciejewski, R. A. Koeppel, R. Tschan, A. Baiker, J. Phys. Chem. 100, 20006 (1996). [3] J.M. Porrás-Vázquez, P. R. Slater, Fuel Cells 12, 1056 (2012). [4] T.J. Huang, X.D. Shen, C.L. Chou, J. of Power Sources 187, 348 (2009). [5] Y. Mastrokov, S. Guo, F. Puleo, L.F. Liotta and E. Kotomin, manuscript in preparation.

**#123 - Electrode-Electrolyte Compatibility in Solid-Oxide Fuel Cells: Investigation of the Interface with X-Ray Microspectroscopy***Marianna Gambino - Dipartimento di Fisica e Chimica, Università di Palermo**Other Authors: Francesco Giannici (Dipartimento di Fisica e Chimica, Università di Palermo, Palermo, Italy), Giovanna Canu (Istituto per l'Energetica e le Interfasi (CNR-IENI), Consiglio Nazionale delle Ricerche, Genova, Italy), Alessandro Longo (Istituto per lo Studio dei Materiali Nanostrutturati (CNR-ISMN), Consiglio Nazionale delle Ricerche, Palermo, Italy), Murielle Salomé (European Synchrotron Radiation Facility, Grenoble, France), Massimo Viviani (Istituto per l'Energetica e le Interfasi (CNR-IENI), Consiglio Nazionale delle Ricerche, Genova, Italy), Antonino Martorana (Dipartimento di Fisica e Chimica, Università di Palermo, Palermo, Italy)*

Chemical and structural compatibility between materials is a critical point in all-ceramic devices working at very high temperatures: in this respect, the degradation of the cell performance is often the critical factor limiting the working life of SOFC.

LaNbO<sub>4</sub> doped with 2% Ca<sup>2+</sup> (LNC) represents the last real breakthrough in the field of proton-conducting oxides for use as electrolytes in SOFC, showing improved stability and high conductivity with respect to perovskites [1]. To develop efficient and robust devices based on LNC, the electrical performance and chemical compatibility of various electrode materials with LNC was extensively tested in recent literature. [2]

We recently applied X-ray microspectroscopy to evaluate the chemical and local structural fate of cations interdiffusing across an LNC/cathode bilayer (where the cathode is either La<sub>0.6</sub>Sr<sub>0.4</sub>MnO<sub>3</sub>, La<sub>0.6</sub>Sr<sub>0.4</sub>Co<sub>0.8</sub>Fe<sub>0.2</sub>O<sub>3</sub>, etc.) after prolonged annealing at high temperatures (1150 °C), to simulate the operating conditions of a fuel cell. The interfaces of the devices were studied with space-resolved X-ray absorption spectroscopy (XAS) using the focused submicrometer-sized beam available at the SXM-II endstation on the ID21 beamline of ESRF. We collected microXANES and microEXAFS spectra at the Nb L<sub>3</sub>, La L<sub>3</sub>, Ca K, Fe K and Mn K edges. The microXRF composition maps spectra were also collected, giving information on the distribution of cations.

In general, an unexpected and impressive exsolution of the Ca<sup>2+</sup> dopant from the LNC electrolyte towards the cathode is observed in all samples. [3] The Ca and Nb change of coordination number and geometry between the perovskite cathode and the LNC electrolyte is well supported by microXANES simulations, pinpointing the greater structural flexibility of the perovskite structure as the driving force behind the incorporation of cations from the electrolyte. Fe and Mn edge microXANES spectra also show interesting variations as a function of the distance from the interface, hinting at some kind of oxygen vacancy accumulation at the interface. At the La, Fe and Mn edges, high quality microEXAFS spectra were collected and modeled up to about 8 Å<sup>-1</sup>.

The present results represent the first application of microfocus X-ray absorption spectroscopy to the study of materials compatibility in SOFC. This approach can be extended to other kinds of electrode materials, including ceramic anodes, cermets, and oxide-ion conductors, reproducing different working conditions of real devices: this is expected to give unprecedented insight on the mechanisms governing electrolyte-electrode compatibility and electrochemical performance in solid oxide fuel cells.

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#### #124 - Toward a new hybrid proton conductor: lanthanum niobate layered perovskites as a source of tailorable surfaces

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The modification of metal oxide surfaces with organic moieties has been widely studied as a method of preparing organic-inorganic hybrid materials for various applications. Among inorganic oxides, the ion-exchangeable layered perovskites [1], materials composed by perovskite-like slabs and intercalated cations, stimulated authors' interest in reason of some encouraging electronic and reactive properties. In particular it is well known that the interlayer surface of such materials in their protonated form can be easily functionalized with organic groups (such as alcohols [2-3] or organophosphonic acids [4]) thus allowing the production of stable hybrid materials with new electronic and reactive features.

Starting from our previous results on the inorganic substrate HLaNb<sub>2</sub>O<sub>7</sub> (HLN) [5], as a further step in the design of new inorganic-organic hybrid proton conductors, the study of some intercalated compounds is here presented, both from an experimental (synthesis and characterization) and a theoretical viewpoint (geometrical and electronic structures). A general very good agreement with the available experimental data has been found in reproducing both structural features and <sup>13</sup>C-NMR chemical shifts.

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#### #125 - Al-foam based composites for metal supported SOFC with improved resistance to degradation

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Solid oxide Fuel Cells are approaching commercial exploitation thanks to joint efforts by research institutions and industries. Such a combination profits from scientific advancements in materials design and optimization. At the moment, research is targeting the recognized limitation of SOFC, basically consisting in excessive performance degradation over the expected lifetime of devices. Several innovations have been explored to overcome such limitation by reducing operating temperature and improving stability of materials.

Second generation cells, anode-supported, make extensive use of Ni as catalytic material for H<sub>2</sub> oxidation reaction, while third generation cells, metal-supported, are commonly fabricated with Ni foam as support. Due to this reason, both types suffer from conductivity loss on redox cycling and exposure to fuels with higher S content, as in biogas.

One possible approach to significantly reduce or completely avoid the use of Ni is the development of a new kind of support made of an Al-forming foam impregnated with an electronic conducting ceramic phase.

Within the European project EVOLVE, a combination of NiCrAl foam and n-doped SrTiO<sub>3</sub> are being studied as potential substrates for metal supported SOFC, with the aim to realize a composite with high resistance to oxidation and good conductive properties.

The properties of single components, the compatibility among different phases and the behaviour of composites under RedOx cycling are reported.

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**#126 - Non-equilibrium quantum manipulation: from robust entanglement to quantum thermal machines**

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We will discuss the behavior of one or more elementary quantum system (atom, molecules, quantum dot, ...) interacting with a stationary, simple and rich electromagnetic environment out of thermal equilibrium: The electromagnetic field is produced by a simple configuration of macroscopic objects held at thermal equilibrium at different temperatures. We will show how the internal atomic dynamics can be deeply affected by the non equilibrium configuration leading to unexpected phenomena like a spontaneous inversion of population, new cooling mechanisms obtained by heating the system, and the possibility to create and protect entanglement in a stationary and robust way. Finally, we will discuss how this system may directly allow the realization of atomic quantum thermal machines, with high efficiency and a genuine quantum behavior.

**#127 - Quantum vacuum experiments in microwave resonators**

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In so-called *dynamical Casimir effect experiments* [1-3] lies the possibility to convert the quantum vacuum fluctuations into directly observable real photons. Non-adiabatic, time-dependent boundary conditions are imposed to the vacuum state of the electromagnetic field in a 3D microwave cavity to accomplish parametric amplification of the initial vacuum or thermal fluctuations.

Two different experimental approaches will be presented that are aimed to the observation of the DCE in three-dimensional, empty cavities, in which the electromagnetic field boundary conditions are altered electronically or by means of ultrafast laser pulses.

Initially it was expected [1] that real photon generation could take place in a three dimensional cavity when the conductivity of a semiconductor slab was optically modulated at twice the fundamental cavity frequency [2], but such experiment has finally been demonstrated to be severely limited by microwave absorption phenomena in the laser-excited semiconductor.

A variable capacitance diode (varicap) located inside a resonant cavity has instead allowed us to initialize a parametric amplification process of the thermal photons of the cavity at finite temperature.

A method to test the apparatus for detection of the quantum photons will be presented, in which the behavior of the thermal radiation in the cavity mode kept at different temperatures  $T$  is investigated, through the study of the coarse-grained energy distribution in the amplified cavity mode [5].

We will also discuss the feasibility of an idea for parametric amplification of the quantum fluctuations that is based on the modulation of the index of refraction of a nonlinear crystal enclosed within a cavity. In this case the process of parametric generation is related to the third order nonlinear coefficient of the nonlinear crystal while the second-order nonlinear coefficient represents a source of spurious photons, which can arise during the process of laser excitation.

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**#128 - Casimir-Lifshitz force out of thermal equilibrium between dielectric gratings**

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*Other Authors: Antonio Noto (University of Montpellier and University of Palermo), Riccardo Messina (University of Montpellier), Mauro Antezza (University of Montpellier)*

We calculate the Casimir-Lifshitz pressure in a system consisting of two different one-dimensional dielectric lamellar gratings having two different temperatures and immersed in an environment having a third temperature. The calculation of the pressure is based on the knowledge of the scattering operators, deduced using the Fourier modal method. The behavior of the pressure is characterized in detail as a function of the three temperatures of the system as well as the geometrical parameters of the two gratings. We show that the interplay between nonequilibrium effects and geometrical periodicity offers a rich scenario for the manipulation of the force. In particular, we find regimes where the force can be strongly reduced for large ranges of temperatures. Moreover, a repulsive pressure can be obtained, whose features can be tuned by controlling the degrees of freedom of the system.

Remarkably, the transition distance between attraction and repulsion can be decreased with respect to the case of two slabs, implying an experimental interest for the observation of repulsion.

### #129 - The experiment PVLAS for the measurement of the magnetic birefringence of the vacuum

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Vacuum magnetic birefringence refers to the changes of the polarization of a light beam propagating in a transverse magnetic field in vacuum. Anisotropies of the index of refraction of a magnetized vacuum are predicted by quantum electrodynamics, but this effect is so small that has yet to be observed. The experiment PVLAS has been designed to detect such effect by using a very sensitive ellipsometer based on a high finesse Fabry Perot cavity. The PVLAS collaboration is presently running a new apparatus in Ferrara (Italy) and the new magnetic source is a pair of 2.5 T, 0.9 m long permanent magnets. In the talk details will be given on the detection technique and the results obtained with the new apparatus. The challenging goal has not yet been reached due to excess noise which is under study. Nonetheless new limits on vacuum magnetic birefringence have been recently set and measurements are still underway.

### #130 - Resonance interaction between two uniformly accelerating atoms

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We consider the resonance interaction between two uniformly accelerated identical atoms prepared in a symmetric or antisymmetric correlated state, interacting with the quantum electromagnetic field in its vacuum state. The atoms are assumed to accelerate in the same direction perpendicular to their separation.

We evaluate the interatomic interaction, separating at the second order in perturbation theory the contributions of vacuum fluctuations and radiation reaction field.

We show that Unruh thermal fluctuations do not affect the interatomic interaction, which is exclusively given by the radiation reaction contribution.

Also, we find that, beyond the characteristic length scale associated to the breakdown of a local inertial description of the two-atom system, non-thermal effects in the radiation reaction term change qualitatively the distance-dependence of the resonance interaction.

### #131 - Three-body radiative heat transfer and Casimir-Lifshitz force out of thermal equilibrium

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A striking consequence of quantum electrodynamics is the existence of an electromagnetic force between any couple of neutral polarizable bodies even in the vacuum state of the electromagnetic field. This effect, known as Casimir effect, was first theoretically predicted in 1948. In 2005 it was shown that the absence of thermal equilibrium deeply modifies this effect, producing quantitative and qualitative differences, such as the appearance of new asymptotic behaviors and the possibility of a repulsive force. The out-of-equilibrium scenario brings to the attention a different closely related effect, the radiative heat transfer. My talk addresses the combination of the absence of thermal equilibrium with three-body interactions. To this aim I discuss a recently developed general theory describing Casimir force and radiative heat transfer in a system consisting of three arbitrary bodies held at three independent temperatures and immersed in a thermal environment. As an application, I consider the force acting on an atom inside a planar cavity. I show that, differently from the equilibrium configuration, the absence of thermal equilibrium admits one or more positions of minima for the atomic potential, paving the way to a possible trapping scheme for Rydberg atoms.

### #132 - Vacuum energy densities of a field in a cavity with a mobile boundary

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Vacuum energy densities of a field in a cavity with a mobile boundary

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**Abstract.** We consider the zero-point field fluctuations, and the related field energy densities, inside a one-dimensional and a three-dimensional cavity with a mobile wall subjected to a harmonic potential. The mechanical degrees of freedom of the mobile wall are described quantum mechanically, and they are fully included in the overall system dynamics. In this optomechanical system, the field and the wall can interact with each other through the radiation pressure on the wall, given by the photons inside the cavity [1] or even by vacuum fluctuations. We consider two cases, the one-dimensional electromagnetic field and the three-dimensional scalar field, and use the Green's functions formalism [2]. We show that the quantum fluctuations of the position of the cavity's mobile wall significantly affect the field energy density inside the cavity, in particular at the very proximity of the mobile wall. The dependence of this effect from the ultraviolet cutoff frequency, related to the plasma frequency of the cavity walls, mass and frequency of the harmonic potential is discussed in detail. We also compare our results for the one-dimensional electromagnetic field and the three-dimensional massless scalar field to results recently obtained for the one-dimensional massless scalar field [3]. Finally, we discuss how the presence of a mobile wall changes the Casimir-Polder force on a polarizable body placed inside the cavity, giving the possibility to detect experimentally the new effects we have considered.

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### #133 - On the impact of dissipation on dispersion interactions between two atoms

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We consider the interaction between two neutral atoms in the presence of an arbitrary arrangement of dispersing and absorbing magnetodielectric bodies by means of a dynamical approach. Our result differs from the previous ones obtained with time-independent perturbation theory because it accounts for the influence of dissipation via the atomic decay rates. Modern measurements of Casimir force seems to indicate an agreement with plasma model instead of Drude model. This has lead to heated debates, because the latter is more a more realistic description of matter. Our new result can explain the agreement with the plasma model for finite temperature. Further investigations will be needed in order to include many-body interactions. In the second part of the article we consider the interaction between a ground-state atom and an excited atom at zero temperature. In the literature there are open debates regarding the retarded limit of the interaction; with the introduction of the decay rates we can solve this debate. Our oscillating result, with respect to the distance, seems go into the same line with recent measurements of the Casimir force between an excited barium ion and a mirror.



**#134 - Rapid CVD synthesis of large-crystal graphene and van der Waals heterostructures**

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Following the remarkable fundamental research of graphene performed using micron-sized mechanically exfoliated flakes, the attention is now turning towards practical applications, and, large-scale synthesis of graphene and related 2D materials is becoming increasingly relevant. Along with thermal decomposition of silicon carbide, chemical vapour deposition (CVD) on metal substrates has become the most widely-used technique to produce large-scale samples of graphene. In particular, CVD growth on copper allows the synthesis of high-quality monolayer graphene, however, the presence of grain boundaries in the typical samples of CVD-graphene as well as the need to transfer graphene to other, non-conductive substrates, remain serious obstacles towards the use of this material for certain electronic and photonic applications. In order to avoid grain boundaries, CVD growth of single-crystal graphene has attracted particular attention in the last few years. While millimetre-sized crystals have been produced by several groups [Hao *et al.*] [Chen *et al.*] [H. Zhou *et al.*] [Yan *et al.*] [Gan *et al.*], the CVD synthesis of such crystals typically involves in-situ oxidation [Hao *et al.*] and resulting safety concerns or requires many hours due to the relatively slow growth rates [Chen *et al.*] [H. Zhou *et al.*] [Yan *et al.*] [Gan *et al.*]

We have recently shown a simple pathway towards rapid synthesis of mm-sized single crystals of graphene using a commercially-available cold-wall CVD reactor [Miseikis *et al.*]. Due to the high growth rates, crystals of up to 3.5 mm can be synthesised in 3 hours. The key steps of the process are: i) using (ex-situ) passivated Cu foils, ii) annealing in an inert argon atmosphere, and iii) enclosing the sample during growth. By using dry and etchant-free transfer techniques, the large single crystals of CVD-graphene can be removed from the metallic growth substrate and transferred to the substrate of choice while retaining the high quality, with electronic characteristics comparable to mechanically-exfoliated flakes. Our large crystals of CVD-graphene transferred on Si/SiO<sub>2</sub> substrates demonstrate a clear quantum Hall effect and field effect mobility above 10 000 cm<sup>2</sup>/V s.

Due to its 2-dimensional nature, the properties of graphene are greatly influenced by the underlying substrate. Hexagonal boron nitride (h-BN) has been known to be the ideal substrate for graphene due to the atomic flatness and low lattice mismatch. However, direct synthesis of graphene on h-BN is still in its infancy and high growth rates (i.e., > 100 nm/min) require complex steps, such as the introduction of gaseous catalysts (e.g., germane and silane) during growth [Tang *et al.*]. In contrast, we show that by optimising the growth temperature and pressure, catalyst-free growth rates higher than 100 nm/min can be achieved on well-prepared bare h-BN substrates [Mishra *et al.*, submitted], thus greatly simplifying the process.

**#135 - The route to the silicene field effect transistor**

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Silicene, a honeycomb-like Si lattice, has been so far a fascinating theoretical surmise [1] with no experimental counterpart as due to the natural sp<sup>3</sup> hybridization of Si bonding. Being an atomically thin layer of silicon, silicene attracts an enormous interest as emerging research material for the semiconductor technology roadmap and for its intrinsic affinity with the ubiquitous silicon technology. Artificially forcing the silicene lattice was firstly made possible in the epitaxial growth of a Si monolayer on Ag(111) substrates [2]. However, unlike graphene, silicene self-organizes in regularly buckled lattices with periodic atomic arrangements as due to the commensurate match with the hosting Ag substrate [3]. This structural complexity results in an interplay of sp<sup>2</sup> and sp<sup>3</sup> bonding which causes the silicene lattice to degrade under environmental conditions. Nonetheless, the hallmark of the silicene lattice can be well-recognized by Raman spectroscopy [4]. The stability and the interaction with the substrates are the two bottlenecks for the "portability" and the exploitation of silicene in device applications. We here exposed effective methods to address both issues and then integrate a silicene layer in a field effect transistor operating at room temperature [5]. In detail, Ag-supported silicene is synthesized on cleavable substrates and then encapsulated for subsequent delamination and transfer into a device-friendly platform. Native Ag is utilized to pattern transistor contacts. The transfer characteristic of the transistor is then measured therein manifesting an ambipolar behavior in close similarity with the graphene behavior. The transport characteristics, the stability issues, and further perspectives are discussed.

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**#136 - Optical response of a composite graphene-Au plasmonic system**

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We report on the optical response of a hybrid graphene/plasmonic device consisting of a 2-dimensional gold nanoparticles (NPs) array coated with a single-layer-graphene foil. The Au NPs, with typical size below 20 nm, are arranged as very-closely-spaced NP chains coherently orientated on a nanopatterned surface, and exhibit a strong absorption of electromagnetic (EM) radiation at  $\lambda=580$  nm, indicative of a localized surface plasmon resonance (LSP).

Large foils of single-layer graphene were fabricated by chemical vapour deposition on Cu foils, then transferred intact onto the Au-NP nanopatterns in aqueous solution. Graphene lies in direct contact with the Au NPs, and acquires a marked uniaxial corrugation due to the morphological influence of the underlying Au-NP chains, that remain intact, in shape and spatial arrangement, following the graphene deposition (Fig.1).

The unique electronic properties of graphene in EM-near-field coupling with the plasmonic particles significantly perturb the local distribution of electromagnetic field intensity, hence the plasmonic response. This is manifest as a remarkable LSP-resonance redshift as the graphene layer is transferred onto the gold nanoparticles.

The uniaxial corrugation of graphene lowers the system's symmetry, introducing a marked uniaxial optical anisotropy in the system's plasmonic response, the LSP redshift being weaker/stronger whereupon the polarization of light is transverse/parallel to the graphene corrugation. This behavior can be understood in terms a corrugation-induced anisotropic conductivity of graphene, that is reflected upon the graphene-mediated interaction between plasmonic NPs.

This finding paves the way to model the high-frequency corrugation-dependent electronic response of graphene and its mechanisms of interaction with plasmonic systems, possibly allowing to tailor the plasmon/graphene hybrid systems' optical response.

**#137 - Band gap engineering through strain in Black Phosphorus Multilayers**

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In this work we study the effects of strain on band gap in black phosphorus multilayers. The peculiar puckered structure of the material leads to strong anisotropy in both electronic<sup>[1],[2]</sup> and mechanical<sup>[3]</sup> properties. Indeed, Young modulus and Poisson ratio in the armchair direction are almost one third of the value in the zigzag direction, producing a mechanical response of the material heavily dependent on the direction of the applied strain. On the electronic side, the effective masses are also extremely different in the two directions resulting in strongly anisotropic transport and optical properties. We start from the analysis of the effects of uniform uniaxial strain on band gap in the two principal direction of the crystal, observing that positive strain produces an enhancement of the gap while on the contrary a negative strain reduces it, leading possibly to its closure for a sufficiently big value of the applied stress<sup>[4]</sup>. This trend is similar in both monolayers and multilayers. We then study the effects of non-uniform strain. By means of prestressed rubber-like substrate we apply a definite stress to mechanically exfoliated black phosphorus in order to create a regular stressed pattern in the lattice. We predict from the existing tight binding model that the sine-like strain profile will lead to a similar pattern in band gap. This prediction is supported by experimental evidence, as emerges from the performed measurements of local optical properties.

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**#138 - Biphenylene: a building block for 2D graphene-like gap-provided molecular network**

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Covalently-bonded 2D carbon networks are graphene-inspired materials, which can combine the outstanding properties of graphene with other important characteristics like, for example, an intrinsic band gap, whose lack in graphene puts severe limits on its applications.

The most reliable technique to grow this kind of materials is a bottom-up procedure, exploiting the surface-confined self-assembly of functional molecular building blocks, used as precursors. Their interaction with appropriate surfaces (generally coinage metals) induces an ordering of the precursors in molecular networks of specific design.

Biphenylene is a cyclic hydrocarbon that can be regarded as the very initial precursor of a 2D porous graphene-like molecular network, called biphenylene carbon (BPC). Density Functional Theory (DFT) calculations demonstrated that BPC is characterized by nonzero band gap and by bands with good dispersion and delocalized frontier orbitals [1, 2], so it could be an ideal structure for many electronic applications.

In order to study the behavior of biphenylene as precursor directly on a surface, in this work we show an x-ray photoemission and absorption (XPS and XAS) investigation on biphenylene films, deposited on a Cu(111) crystal. The occupied core and valence levels and the non-occupied states of the film are examined, to study the electronic properties of biphenylene in solid phase. Considering the importance of the biphenylene-substrate interaction in 2D molecular network formation, the film has been investigated in the multilayer and monolayer coverages to clarify the intermolecular (multilayer) and molecule – substrate (monolayer) dynamics. The obtained results have been compared with spectra of the single biphenylene molecule, provided by gas phase measurements and DFT calculations [3]. This allowed to evidence the modifications induced in the film molecular electronic structure due the molecule–molecule and the molecule–substrate interactions. Furthermore, we have performed a XAS study of the overlayer orientation, whose knowledge is crucial for implementing thin film molecular electronics.

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### #139 - Large-scale Manufacturing of Graphene and Related Materials Inks for Flexible (Opto)electronics

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Graphene and related materials (GRMs) hold great potential for flexible (opto)electronics for their novel electrical, optical and mechanical properties. The road to realistic applications and commercialization of GRMs requires the assessment of three key factors: cost/performance, mass-production and manufacturability with respect to commercially available alternative solutions. For example, transparent conducting oxides used in displays are brittle, printable metal nanoparticles for interconnects are not cost-effective and have demanding processing requirements, while organic polymers are expensive and have limited stability. Low temperature production and deposition of GRM-based inks is thus an attractive alternative for large-area printable, flexible (opto)electronics. GRM inks enable a large range of device fabrication and integration options, such as digital and lithographic printing, roll-to-roll coating, as well as being ideal for embedding into polymer composites or other nanomaterials. Liquid Phase Exfoliation (LPE) of bulk precursor layered materials (such as graphite, MoS<sub>2</sub> crystals, etc.) is a scalable approach ideally suited to produce inks. However, currently LPE has low yield, resulting in a low concentration of dispersed GRMs. I will give a brief overview about the development of high-yield, cost-effective and large-scale production techniques for GRM-based inks, and the portfolio of reproducible manufacturability processes enabling future GRM-based printable and flexible (opto)electronic devices and composites. I will demonstrate cost-effective, up-scalable production of high concentration graphene inks with tailored properties (on-demand size, shape, number of layers and concentration) [1]. By combining LPE with ultra-centrifugation, I will show pilot-scales to produce stable GRM inks through engineered exfoliation and chemical treatment protocols. Fine tuning of the size and shape of the flakes enables the formulation of inks, tailored for various printing and coating methods, such as inkjet, flexographic and screen printing, spray and rod coating. Their distribution of the GRM flakes and their interaction with the substrate controls the final (opto)electronic properties of the printed devices. I will discuss realistic pathways to commercialization of GRM inks and demonstrate prototypes such as: inkjet-printed graphene thin-film transistors [3], flexible transparent touch pads and photodetectors. Finally, I will present my vision on manufacturability of flexible and wearable electronic and optoelectronic devices embedding the optical, electronic, mechanical and thermal functionalities of graphene, 2d crystals and their hybrid hetero-structures.

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### #140 - Studies of the decomposition process of HKUST-1 metal-organic framework (MOF) upon exposure to air

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Metal-organic frameworks (MOFs) are porous crystalline materials with high superficial area, whose structure consists of metal groups connected each other by organic linkers. One of the most studied MOF is HKUST-1, also known as  $\text{Cu}_3(\text{BTC})_2$ . In this material two copper ions are coordinated by four carboxylate groups to form a paddle-wheel motif; these carboxylate groups are the terminal groups of 1,3,5-benzene tricarboxylate (BTC) linker molecules. Both copper ions of the paddle-wheel can establish a fifth coordination bond with small molecules in the immediate environment, especially with small molecules as water. This bond metal site makes the MOF HKUST-1 extremely efficient in the process of adsorption of many small molecules and, consequently, it is the basis of the properties which makes HKUST-1 particularly interesting for many applications.

Studies on magnetic properties of HKUST-1 have shown that the two  $\text{Cu}^{2+}$  ions of the paddle-wheel, each having an unpaired electron with spin  $S=1/2$ , are weakly coupled through a super-exchange interaction involving carboxylate bridges. This leads to the observation of an EPR signal related to a triplet centre ( $S=1$ ) originating from the coupling of the two spins. Furthermore, experiments focused on prolonged exposition of HKUST-1 to water vapour have also pointed out the occurrence of a hydrolysis process that induces a structural decomposition of the paddle-wheels.

In our experiment, we have studied the effect of exposition of a sample of HKUST-1 in powder form to air for different times and we have monitored its structural and magnetic properties by XRD analysis and EPR spectroscopy, respectively. In the first 20 days of the experiment we have recognized a significant reduction of the EPR triplet signal. For longer times of exposition to air a first step of the hydrolysis process takes place causing the break of many Cu-O bonds. This process induces a new arrangement of the paddle-wheel geometry, evident in EPR signal properties, with a small swelling of the crystalline structure. A second step of the hydrolysis process takes place after about 50-60 days of exposition to air and it involves further structural changes of the paddle-wheels. After this last stage about 80% of the matrix has loosed its crystalline order and the decomposition process almost exhausted. This experiment allowed us to examine in depth the knowledge of structural decomposition process of HKUST-1 for exposition to air.

#### #141 - Structural and chemical stabilization of epitaxial silicene on Ag(111)

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Recently, the integration of silicene, the Si counterpart of graphene, in a transistor architecture represented the apex of a deep characterization of this fascinating synthetic 2D material [1]. The route towards its full exploitation in electronic devices goes through an intense work of synthesis of silicene superstructures and their in-situ and ex-situ investigation [2, 3]. Epitaxial honeycomb Si layers have been experimentally observed with non-trivial atomic arrangements, resulting in a polymorphic nature of silicene due to its buckled nature, i.e. the vertical distortion of the honeycomb lattice, which is expected to alter many physical and chemical properties. The basic concepts of the epitaxial silicene growth on Ag(111) by means of a systematic in-situ scanning tunneling microscopy/spectroscopy investigation are here discussed. In particular, attention is devoted to the silicene superstructures phase diagram and to the temperature-driven phase transitions by means of post-deposition annealing processes, which allow manipulating the silicene properties [4]. On the other hand, in the absence of kinetically limited conditions, dewetting takes place and results in a stable silicene multilayer. Moreover, in an applicative view, the process for silicene encapsulation is presented in order to prevent easy oxidation in ambient conditions thus enabling for the transistor realization. These findings disclose exceptionally novel issues in the physics of the silicene and promote a renewed interest in Si at the 2D limit as active material for electronic devices.

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**#142 - POLYMER NANOFIBERS: NEW BUILDING BLOCKS FOR PHOTONICS AND ENERGY-HARVESTING**

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Active electrospun nanofibers are attracting building blocks for a variety of fields, such as optoelectronics, photonics, energy harvesting, nanoelectronics, and microelectromechanical systems [1-4]. In addition, electrospinning technologies can be easily up-scaled to industrial level. Demonstrated device and applications include sub-wavelength optical waveguides and plastic nanofiber lasers [5-7], pressure-sensors, accelerometers and wearables made of piezoelectric polymer nanofibers [8, 9]. Next-generation electrospun nanosystems can be designed and developed, which couple opto-mechanical properties through proper molecular components [10].

Here our recent results on active electrospun polymer nanofibers will be reviewed and discussed. Investigated properties include light-confinement, optical losses, stimulated emission, and anisotropy through emission polarization. Applications in advanced photonics and energy-harvesting wearable technologies will be presented and discussed. The research leading to these results has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013)/ERC Grant Agreement n. 306357 (ERC Starting Grant "NANO-JETS", [www.nanojets.eu](http://www.nanojets.eu)).

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**#143 - Unusual 3D pyro-printing approaches for fabrication of polymeric photonic microstructures**

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The term "pyro-fluidic platform" would express the ability of working on fluids (liquid and/or polymer) exploiting the pyro-electric effect activated onto a ferroelectric crystal in an electrode-less configuration. The no-contact self-assembling of liquids in plane (1D), using a micro-engineered crystal is described while additional degrees of freedom are added improving the dispensing capability and the transfer of material between two different planes (2D) and the controlling and fabrication of three-dimensional structures (3D). The simplicity of the method proposed, associated with the flexibility of the process for fabricating 3D polymer microstructures, demonstrates its great potentiality exploitable in many fields, from optics to biosensing. Furthermore, the manipulation of polymer in combination with the high resolution of the dispensing at nanoscale suggests innovative and potential uses for in situ and non-invasive instruments. In fact, the possibility of manipulating polymers through a nozzle-free approach would be of great interest for the fabrication of micro-structures also for photonic applications. The application of the pyro-electrohydrodynamic approach is applied for the fabrication of polymer microlens arrays, highly ordered patterns of polymer fibers and 3D micro-optical elements (wires, needles, pillars, cones, or microspheres). Micro-axicons have been realized and used for generating Bessel beams (used as optical tweezers in microfluidics). Spherical polymer beads are another class of micro-optical elements and can be used as either passive or active whispering gallery mode (WGM) resonators for label-free detection of biosamples by classical evanescent field coupling; they can also be used as remotely excitable, active, microstructures if they are embedded with dye or quantum dots. In terms of micro-engineering the optical properties of this micro structures it would be possible to combine the use of a biopolymer and the 3D lithography approach to define a smart way of fabrication of biodegradable active microaxicon that as optical microelements could be inserted in lab-on-chip devices. Furthermore the microstructures produced could be used for collecting or distributing light signals in optofluidic devices as potential optical waveguides.

**#144 - INK-JET PRINTING OF GOLD NANOPARTICLES BASED INKS FOR MEDICAL APPLICATIONS**

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Ink-jet printing technology is becoming particularly attractive as an alternative to vacuum photolithography since it takes advantage of the ease of use, the speed, the low processing temperatures, the reduced amount of toxic wastes and the reduced cost. Metal nanoparticles suspensions (nanofluids) seem to have the most promising prospects for creation of novel ink-jet printing materials

for applications in thermal and electrical treatments also for biomedical applications. Among the metal nanoparticles, gold nanoparticles (GNPs) are particularly promising for nano-medicine applications. Moreover, it is possible to exploit spectroscopic features of non-spherically symmetric GNPs that have large Near Infrared (NIR) in the range 800-1200 nm absorption and can induce highly localized thermal load for hyperthermic treatments (with a reduced undesired side-effects on skin of the hyperthermic treatments).

This research was devoted to the development of new thermal and/or conductive type of *non-toxic* ink based on anisotropic gold nanoparticles, namely gold nanostars and gold nanocages. Resulted inks were imprinted on polymeric (latex, PET) and paper (PCC and Kaolin coated paper). The NIR irradiation of imprinted patterns printed with different drop size and the temperature increase under irradiation was studied.

The *significance* of this study is that under mild NIR irradiation the hyperthermic effect of GNPs will allow, in perspective, opportunities to develop warming bandages and stickers for treatment of pathologies, for example musculoskeletal chronic pathologies. In addition to the proposed local heating effect of the warming bandages, it is investigated the *transdermal delivery* of drugs released from nanocages due to NIR irradiation.

#### #145 - ORGANIC MOLECULES for QUANTUM OPTICS: Sensing and Communicating at the nano--scale

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Since decades, atoms --- confined in optical lattices or cavities---have been investigated as elements for a quantum network and fundamental models of complex systems. Complementary to this success in atomic physics, the manipulation of quantum systems in the solid state has brought attention to various atom--like structures.

We focus on the extremely versatile case of molecules in a solid state matrix coupled to photonic nanostructures. We here report on the optical properties of single Dibenzoterrylene (DBT) molecules embedded in Anthracene, and provide a thorough characterization of their fluorescence both at room and at low temperature. At cryogenic temperatures, the interaction with the matrix can be frozen, allowing for coherent light--matter interaction. We discuss the integration of single quantum emitters to dielectric and plasmonic architectures for quantum communication and information processes. We finally present our results on the coupling of single molecules to graphene membranes and demonstrate a position sensor at the nanoscale.

#### #146 - Learning from Nature: how white beetles optimise light scattering

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The colours shown by several insects often arise from light scattering by very complex photonic structures rather than selective absorption by pigments. Such structures are the result of optical strategies developed during millions of years of evolution. The bright and iridescent colours shown by certain butterflies and beetles, for example, is obtained through coherent effects which requires ultrathin periodic layers of material. In contrast, a *bright white* colouration is more challenging to achieve, since all colours must be scattered with the same high efficiency. In this case the wave nature of light is not involved in the appearance of the object, and a bright white is achieved only in presence of multiple scattering, for which thicker, high-refractive-index contrast systems are usually required. Nevertheless, the extremely brilliant whiteness shown by the *Cyphochilus* beetle is generated by multiple scattering of light inside the *ultra-thin* scales that cover its body. The intra scale structure is characterized by a dense, nanostructured network of chitin filaments, which seems to be optimised (during millions of years of evolution) to increase the total reflectance, and thus the bright appearance of the beetle, employing as little material as possible[1]. In this work we analysed light transport inside the beetle's scales demonstrating the onset of a multiple scattering regime despite the extremely low thickness of the structure (5-9  $\mu\text{m}$ ). We proved, with static and time-resolved experiments, that the *Cyphochilus* scales show the lowest transport mean free path for low-refractive-index systems ( $n=1.5$ ) reported to date. We found that the crucial aspect of the optimisation of light scattering is the structural anisotropy of the chitin network. We indeed demonstrated that light transport inside the scales is anisotropic, and it is engineered to increment the scattering strength in the direction orthogonal to the scale surface, at expense of the in plane scattering, which is not relevant for the total reflectance.

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#### #147 - Modelling, design and fabrication of silicon-based photonic Vernier devices for the mid-infrared

Benedetto Troia - Politecnico di Bari

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The Vernier effect has been widely used for ultra-high performance photonic refractive index sensing in the near-infrared by means of cascade-coupled ring resonators, Mach-Zehnder interferometers or mixed combinations of such devices. Recently, some research efforts have been carried out in order to extend the operation of photonic integrated devices from the conventional near-infrared wavelength range to the mid-infrared. Indeed, a great number of chemical/biochemical liquid and gaseous species that are worth being monitored because of their harmfulness or biological role, exhibit vibrational and rotational modes that are spectroscopically accessible within the mid-infrared. In this context, we propose a sophisticated, flexible and reliable design flow based on a rigorous mathematical modelling for the design and fabrication of integrated silicon-based photonic devices working in the second regime of the Vernier effect in the mid-infrared wavelength range of 3.7-3.8  $\mu\text{m}$ . In particular, single and cascade-coupled racetrack resonators based on rib and strip waveguides operating around 3.8  $\mu\text{m}$  with insertion loss lower than 1 dB, extinction ratio up to 25 dB as well as Vernier gains of about 20 have been characterized, resulting in the first experimental demonstration of the Vernier effect in the mid-infrared wavelength range. Furthermore, the reproducibility and reliability of the implemented design tool is demonstrated by means of relative errors even lower than 1 % for the most important Vernier device figures of merit and by a graphical comparison among experimental and theoretical Vernier spectra. In conclusion, preliminary sensing functionalities have also been achieved around 3.8  $\mu\text{m}$  by using a polydimethylsiloxane microfluidic channel and perfluorodecalin which is a low-absorption material in the explored mid-infrared wavelength range.

#### #148 - Room temperature organic polaritons propagation towards all-optical logic circuits

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Exciton-polaritons are bosonic quasi-particles arising from strong light-matter interaction between excitons and photons. They have achieved great importance for studies - typically made in planar microcavities (MCs) - on fascinating subjects such as Bose Einstein condensation,<sup>1</sup> superfluidity<sup>2</sup> and quantum vortex,<sup>3</sup> but also for the realization of ultra fast and highly efficient logic devices thanks to their non linear and in-plane propagation properties.<sup>4</sup> Until now room temperature propagation had never been observed due to the ionization of the exciton in inorganic systems. For this reason, organic materials, with their huge oscillator strength, are achieving a great interest for their capability to condense at room temperature.<sup>5,6</sup> However, organic polariton lifetimes are limited by planar MCs growth difficulties when adopting these "soft" materials and it has hindered so far the possibility to observe polariton propagation in a standard planar MC system.

Using a novel device structure, we couple a Bloch Surface Wave (BSW) mode with an organic exciton, observing for the first time polariton propagation at room temperature over ranges of hundreds of microns. Moreover we demonstrate the non linear interaction above a given power threshold which is the first step towards all-optical logic circuits.

The BSW is a propagating mode existing at a Distributed Bragg Reflector (DBR) surface beyond the critical angle. We experimentally demonstrate the formation of a room temperature Bloch Surface Wave Polariton (BSWP) generated between this optical mode and thin organic layers.<sup>7</sup> The group velocity of these polaritons is around 50% the speed of light, i.e. 150 $\mu\text{m}/\text{ps}$ , which is about two orders of magnitude higher than in planar MCs. In addition, during the propagation path, given the exciton counterpart, the polariton energy relaxation is clearly observable. Furthermore, due to the absence of the top mirror - which is necessary in standard planar MC systems - record organic polariton lifetimes (about 1ps) have been achieved.<sup>6</sup> Moreover, resonantly pumping the BSWP, the mode dispersion blueshifts above a given threshold due to non linear polariton-polariton interactions. Regarding logic operation, this finding is an essential condition for the realization of an optical gate, i.e. the basic component of a logic device. Our results open the possibility to create room temperature BSWP polariton circuits with low dissipation and ultrafast data manipulation and transmission rates.

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**#149 - Photonic engineering of THz-frequency quantum cascade lasers**

Miriam Serena Vitiello (I) - CNR-NANO NEST and Scuola Normale Superiore

Terahertz (THz) radiation lies in the region of the electromagnetic spectrum, loosely defined as the 30-300  $\mu\text{m}$  wavelength region that is often called "THz gap". Recent technological innovation in photonics and nanotechnology is now enabling widespread applications at THz-frequencies in a plethora of fields, such as information and communications technology, sensing, medical diagnostics, global environmental monitoring, homeland security, quality and process controls. Most of these applications require systems with targeted sensitivity and specificity, exploiting advanced photonic and optoelectronic device technologies.

In this perspective, high-power, widely tunable micro-sources with controlled and directional beam profiles and high-spectral purity<sup>1</sup>, together with high-speed and high-sensitivity detectors represent a major need. This requires the parallel developments of novel materials and heterostructures, advanced microstructures and plasmonic approaches as well as proper multifunctional THz optical components.

The talk will provide an overview of our recent technological developments of THz-frequency quantum cascade lasers (QCLs), from the development of the first quasi-crystal THz intersubband laser,<sup>2</sup> to novel distributed feedback concepts, exploiting bi-period feedback gratings to control the emission frequency and the output beam direction of a QCL, independently.<sup>3</sup> A final emphasis on microcavity approaches for continuous tuning of THz QCL emission<sup>4</sup> and waveguide adapters for efficient THz radiation out-coupling<sup>5</sup> will be provided.

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**#150 - Generating ultrafast pulses from quantum cascade lasers**

Sukhdeep Dhillon (I) - Laboratoire Pierre Aigrain

Other Authors: F. Wang, K. Maussang, J. Tignon & S. S. Dhillon Laboratoire Pierre Aigrain, Paris, France

The generation of ultrafast and intense light pulses through modelocking is an underpinning technology across the entire electromagnetic spectrum. While semiconductor-based platforms exist for pulse generation in the visible and near-infrared, modelocking of quantum cascade lasers (QCLs) in the mid-infrared and terahertz (THz) ranges has proven to be extremely challenging, despite 20 years of research effort. I will review recent research in this field and illustrate new insights into the generation of short pulses from THz QCLs.

In particular, and contrary to popular belief that a long gain recovery time is required, we demonstrate that the dominant factor for active pulse generation in QCLs is in fact a "THz-gigahertz phase matching" i.e. the synchronization between the propagating electronic microwave modulation and the generated THz pulses in the QCL. This allows the THz pulse to propagate in phase with the microwave modulation along the gain medium, permitting ultrashort pulse generation. This work brings an enhanced understanding of QCL modelocking and will permit new concepts to be explored to generate shorter and more intense pulses in the mid-infrared and THz ranges.

**#151 - Mid- and far-infrared digital holography based on quantum cascade lasers**

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Extension of hologram recording to the infrared (IR) spectrum has attracted a considerable interest since the early stage of holography, due to the intrinsic relaxation of the mechanical stability requirements and to the IR transparency of many materials opaque to the visible radiation. In addition, IR hologram recording benefits from a large field of view and is well suited for measuring optical path variations, since the use of a long wavelength reduces the need for phase-unwrapping algorithms. In the last decade, in the wake of the establishment of digital holography (DH) in the visible range, the development of pyrocameras and focal plane array microbolometers, combined with powerful and highly coherent CO<sub>2</sub> lasers, has finally boosted IR holography: thanks to sensors including 100,000s of pixels as small as few tens of  $\mu\text{m}$  and operating at room temperature, CO<sub>2</sub> laser based DH has proved its potential for practical applications [1].



Although their maximum output power does not compare to that of CO<sub>2</sub> lasers, QCLs appear as interesting sources for IR holography, due to their compactness, their noteworthy spectral purity and to the coverage of the mid-IR spectrum, from 3 to 16  $\mu\text{m}$ , as well as of the THz spectrum, both extremely attractive for imaging. THz waves are e.g. valuable for non-destructive material quality control and homeland security, thanks to their ability to penetrate plastics, ceramics, paper, and clothes, and to their robustness to scattering. Moreover, QCLs can be mounted in an external cavity and tuned on a broad frequency range, which makes them convenient, in particular, for multiple wavelength holographic interferometry.

In this work we report on our recent results of real time IR digital holography based on QCLs and a high sensitivity microbolometric thermocamera. In the mid-IR we acquired speckle holograms of scattering objects and performed holographic interferometry at synthetic wavelengths ranging from 100s  $\mu\text{m}$  to several mm [2]. In the THz range, we demonstrated for the first time the possibility to record and reconstruct THz digital holograms of both static and dynamic scattering objects. In addition, we obtained amplitude and phase images of transparent samples extracted from THz transmission holograms, paving the way to the use of THz waves for one-shot 2D thickness investigation via optical path length measurement [3].

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### #152 - THz imaging with a quantum cascade laser through optical feedback interferometry

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We study the effect of the optical feedback strength on the phase sensitivity in a continuous-wave (CW) imaging based on self-mixing interferometry with terahertz quantum cascade lasers (THz-QCLs). Optical feedback in QCLs, here used to obtain reflection image of a sample as well as the phase profile without ambiguity, is suited for contactless coherent sensing where the wavelength agility and spectral purity associated with QCLs are required. QCLs are characterized by intrinsic linewidth of tens of Hz, potentially limited to the quantum noise, and CW output power of few mW in the terahertz range. Moreover, QCLs are intrinsically stable against optical feedback, tolerating strong feedback level without exhibiting dynamical instabilities, such as mode-hopping, intensity pulsation or coherence collapse, typical of bipolar semiconductor lasers. This unique behavior of QCLs can be ascribed to two main factors: i) the small linewidth enhancement factor ( $\alpha < 1$  in THz-QCLs) with respect to conventional diode lasers, that reduces the number of external cavity modes possibly concurring in destabilizing the CW emission; ii) the absence of relaxation oscillations (class-A laser) owing to high values of photon-to-carrier lifetime ratio (i.e. ultrafast intersubband relaxation time). Also, the inherent sensitivity of the QCL compliance voltage to the optical feedback is ideal for compact and monolithic sensors using the self-mixing approach, since the power modulation can be detected directly as voltage drop across the QCL active region with no need of external detectors. Indeed, the optical feedback interferometry in QCLs does incorporate the detector functionality within the laser cavity itself, and has been extensively exploited for a variety of relevant applications including, but not limited to, phase spectroscopy, in-line laser ablation monitoring, metrology. In this work, we investigate of the phase sensitivity against optical feedback, showing the existence of a feedback threshold for accurate phase signal detection in the THz domain and its potential applicability.

### #153 - New tools for QCL-based THz Spectroscopy

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Optical resonators are well-established tools commonly used in spectroscopy, they have widespread applications over the whole electromagnetic spectrum, while record-level optical finesses were achieved in the visible/near-IR. In this context, the THz portion of the electromagnetic spectrum is still lacking of such tools. One reason is certainly that, for many years, the THz range has been an underexploited region. However, recent advances in generation and detection of THz radiation, as well as the advent of novel THz-emitting laser sources, such as quantum cascade lasers (QCLs), and the constantly evolving technology of new materials, are now making THz light emerge as a new promising frontier for interdisciplinary research areas. However, among the number of different applications of THz radiation, a central role is played by molecular spectroscopy. In order to further increase the sensitivity of a spectroscopic system, high-finesse cavity resonators represent an attractive tool as they give access to much longer interaction lengths between light and absorbing medium, and could also provide a narrow reference for a QCL, allowing a reduction of its free-running linewidth.

We report on two different resonant cavities designs, injected by a continuous-wave quantum cascade laser emitting at 2.55 THz [1]. The two cavities are a V-shaped and a ring shaped resonator, the input/output couplers of both cavities are wire grid polarizers, acting as highly reflective mirrors, and each cavity is equipped with a shifting mirror, in order to tune the cavity length. The achieved ring-cavity finesse is about 63, corresponding to a Q-factor of  $2.6 \times 10^5$ . Due to its geometrical configuration, the V-shaped resonator produces an optical feedback to the QCL, when in resonance. This optical feedback (OF) prevents an accurate finesse measurements, as it broadens the resonance peak profiles. In order to better understand this effect, we injected both the resonators at the same times; the V-shaped cavity is swept across its resonances, while the ring cavity is kept in a position corresponding to the center of a resonance side. In this conditions, any shift of the laser frequency induced by OF will result in a variation of the signal transmitted by the ring cavity. Experimental data have confirmed this effect, that in the future can be exploited for optically locking the QCL frequency to the V-shaped cavity resonance.

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#### #154 - Recent advances in quartz enhanced photo-acoustic spectroscopy based on mid-IR and THz quantum cascade lasers for gas sensing applications

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The detection of traces of chemical species in the gas phase is of considerable interest in a wide range of applications such as environmental air quality monitoring, medical diagnostic, homeland security, quality and process controls. Quartz enhanced photo-acoustic spectroscopy (QEPAS) is a robust and highly sensitive trace-gas optical detection technique. The recent developments of quantum cascade laser (QCLs), mid-IR hollow fibers and quartz tuning forks (QTFs) has allowed to further expand the great potentialities of QEPAS based sensors and reach sensitivities of few parts per trillion [1]. We will report an overview of the latest advances in QEPAS trace-gas sensor technology such as the realization of fiber coupled QCL based sensors operating either in the mid-IR or in the THz spectral range [2]. Results on the realization of newly designed QTFs with improved performances will be also discussed.

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**#155 - Protein-Protein interactions from a co-evolutionary perspective**

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Other Authors: *Christoph Feinauer (Politecnico di Torino)*

Thousands of proteins are simultaneously expressed in a typical cell, and their concerted specific interactions regulate the large majority of cellular functions leading to healthy or diseased states. Two major questions are crucial for our understanding of protein-protein interaction networks: (1) who interacts with whom, and (2) how proteins interact at the structural molecular level. I will present an advanced algorithmic strategy combining a vast array of computational techniques: from statistical physics, to molecular modeling and machine learning. To tackle these challenges, we I will introduce in particular an approach based on residue co-evolution in proteins: evolutionary changes in proteins are constrained by the need to maintain intra- and inter-protein interactions potentially deleterious mutations in one position must be compensated by complementary mutations in other positions, leading to correlated amino-acid occurrences. In particular I will introduce the Direct-Coupling Analysis (DCA) frames co-evolution analysis as an inverse problem in statistical physics. I will provide a systematic evaluation of the information contained in correlated substitution patterns for predicting residue contacts, a first step towards a purely sequence-based approach protein-protein interaction predictions, discussing some relevant example of subnetworks in bacteria.

**#156 - Molecular dynamics simulations of membrane proteins: from the bench to in silico and back**

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The field of classical molecular dynamics simulations has been constantly expanding its range of applications since its origins. The technological breakthroughs in high performance computing techniques have been paralleled by the continuous improvements in the understanding of the simulation algorithms, the parametrization of the force fields and, last but not least, the availability of reliable software. Although this has provided unprecedented possibilities for almost any group in the world, the implicit approximations and generalizations that characterize the method may severely flaw computational studies wishing to investigate extremely complex systems at an atomistic level of detail. As with any other theoretical model, its validity can be assessed only by a direct comparison of its predictions with experiments. In this respect, biological systems represent an even more intriguing challenge: the "quantitative revolution" of modern molecular biology offers the possibility of a direct comparison between simulations and real-time single-molecule experiments, thus contributing to the validation and improvement of the employed force-field parameters. In addition, most experimental groups in biology have accepted MD simulations as a new "tool" that should complement the available experiments and thus offer a direct "view" on a biological process. Therefore, it is nowadays almost mandatory that any molecular dynamics simulation be part of a more comprehensive effort in trying to investigate a complex system, whether biological or not.

In this context, I will present two case studies in which classical MD simulations are employed to provide some insight on two biological systems of interest in our University.

The first is Aquaporin-4 (AQP4), the predominant water channel in different organs and tissues. An alteration of its physiological functioning is responsible for several disorders of water regulation and, thus, is considered an attractive target with a promising therapeutic and diagnostic potential. The application of MD simulations allowed us to describe a new gating mechanism that might be responsible for the narrowing of the pore and thus of a remarkable decrease in water flux rate. We also explored the consequences of different point mutations and compared our results with the experimental observations, obtaining full agreement and a molecular rationale for the observed deviations.

The second is voltage-gated chloride channel, ClC-1, mainly distributed in the skeletal muscle, whose mutations are responsible for the onset of myotonia congenita, a genetic neuromuscular channelopathy. Also in this case, we have shown that a specific mutation (F484L) is responsible for an alteration in Cl<sup>-</sup> gating, in full agreement with the experimental evidence, thus contributing to the formulation of a mechanistic hypothesis for the observed channel malfunction.

**#157 - Improved prediction of protein complex binding affinities: the role of entropic contributions**

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Protein-protein interactions play an essential role in the biological function of many proteins.

We will tackle the problem of predicting the binding affinities of protein complexes, based on the knowledge of both the complex and the unbound subunits. We will rely on the BACH statistical potential, recently developed in our group, and showed excellent performances in discriminating the native states of monomeric proteins.

We will first show that the BACH scoring function is successful as well in recognizing native and close-to-native protein complexes.

We will then employ our scoring function as the basis of a method to predict the binding affinities of protein complexes, which is in general a very difficult task. We will show that, in order to improve the predictive performance of our method, it is crucial to properly estimate how the change in protein fluctuations upon binding determines the entropic contribution to the binding affinity.

This is done by means of simple coarse-grained elastic network models; yet, it relies on determining the proper structure-dependent elastic constant by means of a novel self-consistent procedure based on matching the residue mobilities computed within the network model with those estimated from molecular dynamics all atom explicit solvent simulations initiated from the experimental structures.

**#158 - Adaptive resolution simulation methods in soft matter: theory and applications**

*Raffaello Potestio - Max Planck Institute for Polymer Research*

A feature common to most soft matter systems, ranging from simple liquids to large biomolecules, is the interplay of characteristic length and time scales, which determines their mechanical and dynamical properties. This multi-scale nature limits our capability to study them by means of computer simulations: in fact, the size of the system often makes it impossible to treat the whole of it at the full-atom level; at the same time, coarse-grained models might lack relevant chemical details. An effective solution to this problem is provided by adaptive resolution simulations techniques, which allow the concurrent use of models at different levels of resolution in different regions of the simulation domain. These strategies are here presented, and their application in the computational study of biomolecules is discussed.

**#159 - Variational Scheme for All-atom Characterisation of the Structural Dynamics of Biomolecules**

*Pietro Faccioli - Physics Department University of Trento*

*Other Authors: S. a Beccara (FBK Trento)*

In this talk I would like to report on the recent results of my group in the development and application of path integral based theoretical/computational schemes to investigate rare conformational reactions of biomolecules.

In particular, I would present a new variational approximation which enables us to perform all-atom simulations of complex protein reactions in explicit water, including folding and conformational transitions (see e.g. S. a Beccara, L. Fant and P. Faccioli, PRL 114, 098103 (2015)).

As an illustrative application I will report on our study of serpin latency transitions (Cazzoli et al PNAS ;111(43):15414 (2014)).

Depending on time availability I would finally mention some recent further technical improvements which involves the systematic coarse grain the biomolecular dynamics using Renormalization Group methods.

**#160 - Compilation of a Gene/miRNA Expression Profile Dataset for miRNA:mRNA Interactome Analysis**

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MicroRNAs (miRNAs) are small non-coding RNA molecules mediating the translational repression and degradation of target mRNAs in the cell. Mature miRNAs are used as a template by the RNA-induced silencing complex (RISC) to recognize the complementary mRNAs to be regulated. Up to 60% of human genes are putative targets of one or more miRNAs. Several prediction tools are available to suggest putative miRNA targets, however, only a small part of them has been validated by experimental approaches. In

addition, none of these tools does take into account the network structure of miRNA-mRNA interactions, which involve competition effects crucial to efficiently predict the miRNA regulation effects in a specific cellular context.

We aim to model the miRNA-mRNA interaction network (interactome), by considering all the miRNAs and mRNAs endogenously expressed in any specific cellular condition. Our test bed has been breast cancer MCF-7 cells. We collected several miRNA and mRNA expression profiles, by using the Agilent microarray platforms. We analyzed samples derived from the immunoprecipitation (IP) of two RISC proteins, AGO2 and GW182, and correspondent input and flow-through as well. The expression level of the top expressed miRNAs has been validated by real time PCR.

Due to the singularity of our dataset, we used non-standard bioinformatics techniques to preprocess and analyze the obtained expression profiles. As result, we validated the sample extraction technique, by obtaining expression profile clustering and regression results consistent with the experimental design. The compiled dataset will be useful to further investigate on miRNA-mRNA interactions.

### #161 - Arrested coarsening and localized patterning on curved membranes

*Giulio Vandin - Università di Padova, Dipartimento di Fisica*

*Other Authors: Prof. Enzo Orlandini (Dipartimento di Fisica, Università di Padova), Prof. Davide Marenduzzo (School of Physics and Astronomy, University of Edinburgh)*

The arrest of the coarsening in phase separation dynamics is an interesting feature occurring in several examples of soft matter physics such as bacteria with density-dependent diffusivity and colloidal systems with short range attractive potentials. In this work we focus on a  $\phi^4$  theory of phase separation on closed surfaces (i.e vesicles) in which the free energy of the system includes a term coupled to the local curvature of the membrane. Based on numerical simulations and theoretical considerations we show how the interplay between the bulk term and the surface curvature coupling induces an arrest of coarsening of a binary mixture system in the presence of non-homogeneous curvature and for different closed surfaces. We next consider a reaction-diffusion system of Turing type defined on a substrate undergoing a phase separation similar to the one described above. In this case we show how, by setting different diffusion coefficients for the two phases of the substrate, we can induce a patterning on the closed surface whose shape can be controlled by the curvature of the underlying surface.

### #162 - Codon bias and E.coli's protein-protein interaction network

*Andrea Giansanti - Physics Department, Sapienza University of Rome*

*Other Authors: M. Dilucca, G. Cimini, A. Semmoloni and A. Deiana Physics Department, Sapienza University of Rome*

Synonymous codons, i.e., DNA nucleotide triplets coding for the same amino acid, are used differently across the variety of living organisms. The biological meaning of this phenomenon, known as codon usage bias, is still controversial. In order to shed light on this point, we propose a new codon bias index, CompAI, that is based on the competition between cognate and near-cognate tRNAs during translation, without being tuned to the usage bias of highly expressed genes. We perform a genome-wide evaluation of codon bias for E.coli, comparing CompAI with other widely used indices: tAI, CAI, and Nc. We show that CompAI and tAI capture similar information by being positively correlated with gene conservation, measured by ERI, and essentiality, whereas, CAI and Nc appear to be less sensitive to evolutionary-functional parameters. Notably, the rate of variation of tAI and CompAI with ERI allows to obtain sets of genes that consistently belong to specific clusters of orthologous genes (COGs). We also investigate the correlation of codon bias at the genomic level with the network features of protein-protein interactions in E.coli. We find that the most densely connected communities of the network share a similar level of codon bias (as measured by CompAI and tAI). Conversely, a small difference in codon bias between two genes is, statistically, a prerequisite for the corresponding proteins to interact. Importantly, among all codon bias indices, CompAI turns out to have the most coherent distribution over the communities of the interactome, pointing to the significance of competition among cognate and near-cognate tRNAs for explaining codon usage adaptation.

**#163 - Reaction diffusion patterns on complex directed graphs***Duccio Fanelli (I) - University of Florence**Other Authors: Malbor Asllani (University of Namur, Belgium), Silvia Conemori (University of Florence), Francesca Di Patti (University of Florence), Filippo Miele (University of Florence).*

The process of pattern formation for reaction-diffusion systems is discussed. According to the deterministic picture, partial differential equations are assumed to govern the evolution of the concentrations of the interacting species. A small perturbation of a homogeneous fixed point can spontaneously amplify as follow a symmetry breaking instability and eventually yield asymptotically stable non homogeneous patterns, the celebrated Turing patterns. Traveling waves can also manifest as a byproduct of the instability. Building from these premises, I will discuss in this talk the process of pattern formation on a complex network. In particular I will focus on directed networks: due to the structure of the network Laplacian, the dispersion relation has both real and imaginary parts, at variance with the conventional case for a symmetric network. It is found that the homogeneous fixed point can become unstable due to the topology of the network, resulting in a new class of instabilities which cannot be induced on undirected graphs. A multiple scale perturbative calculation is also carried out resulting in a Stuart-Landau equation for the non linear evolution of the amplitude of the unstable mode.

**#164 - Exactly solvable models for the rate constant of modern nano-reactors***Francesco Piazza (I) - University of Orléans, and Centre de Biophysique Moléculaire (CBM), CNRS-UPR4301**Other Authors: Duccio Fanelli, Università di Firenze Marta Galanti, Università di Firenze and Université d'Orléans*

The recent advances in nano-fabrication processes make now possible to realize many complex nano-catalysts for technological applications. These include vesicle-encapsulated enzymes and core- and yolk-shell composite nano-reactors where many metal nanoparticles or enzymes are immobilized in thermosensitive hydrogel matrices.

It is therefore paramount to build theoretical models that enable one to compute the reaction rate constant of complex nano-catalysts as a function of relevant parameter, such as the ligand diffusion constant, the geometry of the nano-reactor assembly and the transfer free energy from the bulk to the nano-reactor matrix.

In this talk I will illustrate different theoretical approaches toward this aim, based on the solution of stationary diffusion processes with suitable set of complex mixed boundary conditions that describe the reactive boundaries.

**#165 - Optimal search strategies on complex multi-linked networks***Francesca Di Patti - Università degli Studi di Firenze, Dipartimento di Fisica e Astronomia**Other Authors: Duccio Fanelli (Università degli Studi di Firenze, Dipartimento di Fisica e Astronomia and CSDC), Francesco Piazza (Université d'Orléans, Centre de Biophysique Moléculaire)*

This work reports on a major advance in the theory of dynamical processes occurring on complex networks. We focus preliminarily on a general type of random walk, combining with a certain prescribed relative probability both local and non-local moves. Local moves are steps taken along the links of the underlying network. Non-local moves are jumps to randomly chosen disconnected nodes. This kind of stochastic process is a simple yet meaningful model to describe a wide array of dynamical processes on networks, from web-surfing to intra- and inter-layer transport in multi-sheet supports, such as ground/air transportation networks or the brain.

We introduce a global measure of search time, which gauges the overall ability of an agent (e.g. a web-surfer, a traveller or an electric pulse) to find a target at a given location. We show how to compute the search time analytically for a given choice of the starting and target nodes, which can be subsequently averaged over all pairs of nodes to yield a global measure of search effectiveness. Analyses performed on different kinds of synthetic as well as real-world networks show that the global search time displays a minimum for an optimal value of the probability  $\alpha$  to hop along a link (local move) at each time step.

We conclude our analysis by elaborating an analytical criterion that can be applied to any given network to inquire about the existence of an optimal dual-step search algorithm. It is straightforward to employ our simple formula to design the optimal search strategy for any given network, i.e. by specifying a reasonable guess for the relative probability that one needs to assign to local and non-local moves.

These results have been generalized also to multi-linked networks with an arbitrary number of mutually interfering link sets.

**#166 - Turing patterns in multiplex networks***Timoteo Carletti - University of Namur**Other Authors: M. Asllani, University of Namur, Belgium D.M. Busiello, University of Padova, Italy D. Fanelli, University of Firenze, Italy G. Planchon, University of Namur, Belgium*

Patterns are widespread in nature. In the animal kingdom

coloured patterns are the result of adaptation and evolution with the goal to achieve camouflage and social signalling. In chemistry examples are spatial motifs (Belousov–Zhabotinsky reaction), exemplifying a spontaneous self-organization phenomenon. In the seminal paper of 1952, Alan Turing set a plausible and general explanation for the emerge of patterns in reaction–diffusion systems in continuous domains: under specific conditions, diffusion drives an instability by perturbing a homogeneous stable fixed point, via an activator-inhibitor mechanism. As the perturbation grows, non linear reactions balance the diffusion terms, yielding the asymptotic, spatially inhomogeneous, steady state.

In many relevant cases it is more natural to describe the system as a complex network. Examples abound in ecology, the nodes of the networks mimic localized habitat patches, and the dispersal connection among habitats result in the diffusive coupling between adjacent nodes. In the brain a network of neuronal connections is active, which provide the backbone for the propagation of the cortical activity. But also in socio-technological networks, such as the internet and the cyberworld or the commuting networks of human mobility (car, trains, flights). The Turing ideas have been recently extended by Nakao and Mikhailov to random undirected networks, starting from previous works by Othmer and Scriven 1971–1974.

However, the complex network framework can be not general enough to ascertain the complexity that hides behind some real world applications, where self-organization may proceed across multiple, inter-linked networks, by exploiting the multifaceted nature of resources and organizational skills. For this reason, multiplex, networks in layers whose mutual connections are between twin nodes, have been introduced as a necessary leap forward in the modeling effort. In this work we derive for the first time a general theory of patterns formation for multispecies reaction diffusion systems on a multiplex. Cooperative interference between adjacent layers manifests, yielding stratified patterns also when the Turing like instability on each individual layer is impeded. Conversely, patterns on individual layers can also fade away due to cross-talking between layers. The analysis is carried out analytically via a perturbative scheme which enables to derived closed analytical expressions for the critical coupling that determines the aforementioned transitions. In the case of degenerate multiplex networks, namely where all the layers are formed by the same network, we are able to prove that patterns can be created and/or destroyed adding or removing sufficiently many layers. The adequacy of the analytical predictions is confirmed by direct numerical simulations.

#### #167 - Single-File dynamics of colloidal particles in microfluidic channels

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The diffusion of particles confined in a channel so narrow that they cannot overtake each other (Single File condition), a process relevant in Biology and Nanotechnology, reveals nontrivial physical features as a consequence of the strong inter-particle correlations. By means of analytical techniques[1], numerical simulations and experiments performed in microfluidic devices[2], we study the emptying process of  $N$  colloidal particles confined in open channels, i.e. we characterize the progressive decrease of the number of particles within a channel, as they leave it from its open ends.

[1] Phys. Rev. E 91, 022109 (2015)

[2] Lab Chip 11, 3365 (2011)

#### #168 - Self Healing Percolation

*Antonio Scala - CNR - Istituto Sistemi Complessi*

We introduce the concept of self-healing in distribution networks characterised by a flow of services. We define the problem in terms of a distributed message-passing protocol that we analyse both with numerical simulations and with the cavity method. We find that the system is subject to two kind of events: major blackouts and percolative healing. We then generalise the model to a percolation problem that we solve in the case of Erdos-Renyii networks on the complete graph; furthermore, we analyse the two dimensional behavior via numerical simulations. We find that, like in standard 2d percolation, duality rules the transition lines of self-healing percolation on planar lattices.

#### #169 - Protein diffusion, stability and activity in crowded media

*Loredana Randazzo - National Research Council of Italy, Institute of Biophysics*

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Molecular crowding at the cellular level is capable of changing the properties of the macromolecules involved in disparate biological processes and it is thought to affect differently small and large molecules. Here we present a study of ovalbumin and neuroserpin diffusion both in hen egg albumen and in two systems containing ovalbumin and Ficoll70, respectively, to model media with moderate to very high viscosity. These proteins belong to a class of proteins, called serpins, characterized by a high structural homology and different functions. Particularly, neuroserpin, a serine protease inhibitor, is involved in a rare conformational genetic disease (FENIB). We used two techniques for studying different aspects of the molecular motion: Fluorescence Correlation Spectroscopy, that reveals the self-diffusion of particles labeled with a fluorescent probe, and Dynamic Light Scattering, that measures the collective diffusion of all particles, as affected by intermolecular interactions. Moreover we used other techniques for assessing protein conformation: Circular Dichroism, that measures the secondary structure, Intrinsic Photoluminescence, that measures tryptophan exposure to solvent, and continuous-wave Electron Paramagnetic Resonance, that reveals the local mobility of a spin label attached to the protein residue. A cysteine-containing variant of the wild type neuroserpin was produced to get a fluorescently labeled system, without affecting protease inhibition or serpin polymerization. Effects of the crowded environment on both protein diffusion and functional and dysfunctional reaction kinetics were studied.

#### **#170 - Relaxation-path selection due to entropy-energy competition in activated glassy dynamics**

*Chiara Cammarota - King's College London*

*Other Authors: Enzo Marinari, La Sapienza University of Rome, Italy Giulio Biroli, IPhT CEA Saclay, France*

The description of activated relaxation of glassy systems in the multidimensional configurational space is a long-standing open problem. In this talk I will report on my recent numerical and analytical studies of the equilibrium and out-of-equilibrium dynamics of a number of models with rough potential energy landscapes. These models range from abstract trap models to the Random Energy Model (REM) (a paradigm for glass phenomenology) also providing examples of dynamics where typical relaxation channels go over finite potential energy barriers despite the presence of less-energy-demanding escaping paths in configurational space; this phenomenon is naturally expected to be relevant in the thermally activated regime of realistic models of glass-formers. I will show that in the systems we studied typical dynamical paths episodically reach a high fixed threshold energy unexpectedly giving rise to a simple thermally activated aging phenomenology. In order to unveil this peculiar aging behaviour I will introduce a novel description of the dynamics in terms of spontaneously emerging dynamical basins. This result establishes the first quantitative connection between aging in simple and fully solvable thermally-activated systems like trap models and the observed more complex dynamics that could characterise out-of-equilibrium relaxation in realistic glass-like systems.



**#171 - Water clusters, ice and bulk liquid: improving ab-initio structure and energetics**

*Dario Alfe (I) - University College London*

Water in its many forms is one of the most studied of all substances, but in spite of many decades of effort a fully comprehensive account of the energetics of water systems at the molecular level is still lacking. Density functional theory (DFT) is a convenient and important method for water studies, as it can be readily applied to clusters, bulk liquid and solid, surfaces and solutions. However, current implementations of DFT are still lacking satisfactorily overall accuracy. Quantum chemistry (QC) methods like MP2 and CCSD(T) (often regarded as the gold standard) can deliver much higher accuracy than DFT, but they are expensive and scale ferociously with the size of the system, making them available to study only relatively small clusters.

The polarisability of the water molecule means that large clusters, and ultimately extended systems, can behave very differently from small clusters, and so a complete characterisation of the energetics of both small and large systems is required.

An alternative method that has been shown to approach QC accuracy for water clusters energetics is quantum Monte Carlo (QMC).

An advantage of QMC over QC is its benign scaling with system size, and as such it can be applied to large clusters and to bulk solid and liquid.

In this talk I will discuss how it has become possible to use QMC to provide benchmark energies for water systems of various size. I will discuss the limitations of several commonly used DFT functionals, including recent functionals that include dispersion, and possible ways to improve upon them.

**#172 - Subsystem Density Functional Theory for weakly-interacting systems: the role of the Laplacian of the density in the non-additive kinetic and exchange-correlation energy**

*Fabio Della Sala (I) - Istituto Nanoscienze-CNR & Istituto Italiano di Tecnologia (IIT)*

*Other Authors: Szymon Szmiga (Nicolaus Copernicus University, Torun, Poland), Lucian A. Constantin ( CBN, Istituto Italiano di Tecnologia), E. Fabiano (Istituto Nanoscienze-CNR), S. Laricchia (Temple University, Philadelphia)*

Subsystem Density Functional Theory (Sub-DFT) is attracting increasing interest due to its promise of achieving potentially exact results for large systems at a reduced computational cost [1,2,3]. Accurate results have been obtained for weakly-interacting systems [2,3]. However, the accuracy of Sub-DFT depends on the quality of the non-additive kinetic energy (KE) and/or exchange-correlation (XC) functionals, which describe the interaction between subsystems,

We report on newly developed non-additive KE and XC functionals which depends on the Laplacian of the electronic density:

i) We developed new non-empirical Laplacian-level KE functionals [4] which recover the fourth-order gradient expansion (GE4) in the slowly-varying density limit and the APBEK limit [5] in the rapidly-varying density limit.

From tests on weakly interacting systems we found that our new functionals are competitive with state-of-the-art [5], whereas all other previously developed Laplacian-level functionals recovering GE4 fail badly.

ii) We propose a Laplacian-level approximation to the KE density which allow to apply meta-GGA XC functionals in subsystem DFT [6]. Previously, only semilocal XC functionals have been applied to Sub-DFT. Results indicate that a Laplacian term from the second-order gradient expansion of the KE is the best choice and yield very accurate results for weakly-interacting systems.

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**#173 - Wave-like Nature of the van der Waals Energy at the Nanoscale**

*Alberto Ambrosetti - Università degli Studi di Padova, Dipartimento di Fisica e Astronomia*

*Other Authors: Robert DiStasio Jr. (Princeton), Nicola Ferri (Fritz-Haber Institut), Pier Luigi Silvestrelli (Università di Padova), Alexandre Tkatchenko (Fritz-Haber Institut Berlin)*

Wave-particle duality is a cornerstone of quantum mechanics. Given that the ubiquitous van der Waals (vdW) interactions between nanoscale objects have quantum-mechanical origin, it is unsettling that our conceptual understanding of these forces largely relies on models based on localized particles. Here we demonstrate that vdW interactions at nite distances between polarizable nonmetallic nanoscale objects can only be correctly described by wavelike uctuations. The diversity of nanoscale systems, as exhibited by their dimensionality, topology, and polarizability, leads to visibly

enhanced non-local responses and non-trivial vdW interaction power laws that strongly deviate from predictions stemming from widely used intermolecular perturbation theories. Such wavelike nature of vdW interactions provides a hitherto unexplored avenue that could be used for tailoring the assembly of complex polarizable nanostructures.

#### #174 - Electronic Properties of Materials with a Self-Consistent Interatomic van der Waals Density Functional

Nicola Ferri - Fritz-Haber-Institut der MPG

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How strong is the effect of van der Waals (vdW) interactions on the electronic properties of molecules and extended systems? To answer this question, we derived a fully self-consistent implementation of the density-dependent interatomic vdW functional of Tkatchenko and Scheffler [1] and its extension to surfaces [2].

Not surprisingly, vdW self-consistency leads to tiny modifications of the structure, stability, and electronic properties of molecular dimers and crystals. However, unexpectedly large effects were found in the binding energies, distances and electrostatic moments of highly polarizable alkali metal dimers. Most importantly, vdW interactions induce complex and sizable electronic charge redistribution in the vicinity of metallic surfaces and at organic/metal interfaces.

As a result, a substantial influence on the computed workfunctions was found, revealing a non-trivial connection between electrostatics and long-range electron correlation effects [3].

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#### #175 - Molecule-surface interactions: applications in heterogeneous catalysis

Francesca Costanzo - University of Amsterdam

Understanding the reactivity of organic molecules at surfaces plays an important role in surface science. Many applications in catalysis are based on these processes such as light-emitting diodes, molecular sensors and photovoltaics. To tune their electronic properties and functions it is essential to understand the structure and stability of such systems. Density functional theory (DFT), at present, is the most promising approach to study the structure, stability, and electronic properties of complex systems. However, state-of-the-art approximations to DFT do not provide a consistent and reliable description for these systems especially when including metal surfaces, mainly due to two issues: (a) the lack of (long-range) van der Waals (vdW) interactions (b) the spurious self-interaction of the electrons with themselves arising from the Hartree term of the total energy that is not fully compensated in approximate exchange-correlation functionals. The self-interaction errors sometimes lead to an incorrect description of charge transfer and electronic level alignment in these systems, although for molecules adsorbed on metals these effects will often cancel out in total energy differences.

In this talk, I present two applications concerning hydrogen storage. We use DFT+vdW level of theory to model the interaction between hydrogen molecules and graphene, with a particular focus on the effect of the curvature of the graphene surface in carbon nanotubes.

An application in catalysis concerns the oxidation of water on the metal-oxide surface, NiOx. To model the water splitting on NiOx surface, pure and doped with Co, we employ the Hubbard model in the DFT calculations. The catalytic effect of doping the NiOx surface on the splitting of the water is discussed, with the interesting conclusion of reducing the water splitting over-potential by more than 60%.

#### #176 - Thermal diffusion and colored energy dissipation in hydrogen bonded liquids

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Other Authors: Claudio Melis (Dipartimento di Fisica, Università di Cagliari), Michele Ceriotti (EPFL, Lausanne, Switzerland), Davide Donadio (Max Planck Institut für Polymerforschung, Mainz, Germany), Luciano Colombo (Dipartimento di Fisica, Università di Cagliari)

Hydrogen bonded liquids, such as alcohols and water, are characterized by a complex energy dissipation dynamics due to the strong directionality of the hydrogen bonds and the complexity of the hydrogen bonded network. This behaviour impacts the mechanisms of both thermal diffusion and energy dissipation in pump-probe spectroscopy.

By means of out-of-equilibrium classical molecular dynamics simulations we study thermal transport and energy dissipation in liquid methanol. Heat transport is studied by using the "Approach-to-Equilibrium Molecular Dynamics" method, where thermal conductivity is calculated by monitoring the time-evolution of the system temperature profile while it relaxes to equilibrium. Energy dissipation, instead, is studied by means of a novel implementation of the Generalized Langevin Equation (GLE) colored noise thermostat. This is a modified Langevin thermostat, which can generate a non-equilibrium frequency resolved dynamics by using a correlated noise. The colored thermostat can

thermally excite a narrow range of vibrational modes, typically the stretching mode of the OH involved in hydrogen bonding, leaving the other degrees of freedom of the system at the equilibrium temperature. The energy dissipation is then observed as a function of time, by probing the excitation decay and the energy transfer to the other modes.

### #177 - Equilibrium self-assembly of colloidal cubes in the low-density regime

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The self-assembly of colloidal particles is determined by the interplay between competing interactions, usually with energies on the order of the thermal scale. These interactions describe the repulsive and attractive contributions and determine the overall colloidal stability. The contributions can be spherically symmetric or can have an angular dependence. The structure and stability of aggregates is determined by the competitive relationship between all forms of interaction, be they attractive or repulsive, symmetric or anisotropic. Cubic particles are an example of an experimentally realised colloidal system, which can offer the opportunity to study and manipulate these interactions. In order to identify the significance of each contribution to the nature of the self-assembled structures observed, we present here predictions and simulations related to low-density suspensions of cube-like particles. Three distinct systems - with varying inter-particle interactions - have been considered. Namely, a system comprising only van der Waals (vdW) forces, modelled as a standard Lennard-Jones system; secondly, a system with magnetic and steric components, modelled using dipolar and Weeks-Chandler-Anderson potentials; and finally a combination of both interaction types in system three (vdW and magnetic), analogous to a Stockmayer system. Using this methodology, we can attribute the relative importance of each interaction in the combined system, and identify the most important parameters with which to control response functions. In particular, we aim to deconvolute the interplay between the vdW interaction and dipolar interaction during the equilibrium self-assembly of these colloidal particles.

### #178 - Dynamical crossovers in bulk liquid water investigated by molecular dynamics simulations with different potentials

*Marco Sant - Università degli Studi di Sassari*

*Other Authors: Pierfranco Demontis, Marco Masia, Giuseppe B. Suffritti*

The interplay between dynamical heterogeneities and structural properties of bulk liquid water is here investigated by studying the distribution functions of the rotational relaxation constants and the atomic mean-squared displacements.

These distributions are evaluated through molecular dynamics simulations performed with two different potentials: a model developed in our group for the study of nanoconfined water and the TIP4P parametrization.

Two dynamical crossovers are detected from the trend of the Arrhenius plots of the relevant dynamic quantities: the first around 207 K and the second around 280 K. Both potentials give similar results for the dynamical properties, but are markedly different for the structural characteristics.

**#179 - MagnetoHydroDynamics of Optically Thin Astrophysical Plasmas**

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Optically thin plasmas are ubiquitous in the Universe. This presentation addresses some problems related to MagnetoHydroDynamics of astrophysical optically thin plasmas, tackled by some Italian groups; emphasis is on modeling and on High Performance Computing, especially on large computing facilities. Topics range from solar and stellar coronae (i.e. non-thermally heated magnetized plasmas) to jets and accretion flows.

**#180 - Role of laser polarization on stable injection of laser-plasma acceleration at high dose for radiobiology applications**

*Labate Luca (I) - Consiglio Nazionale delle Ricerche, Istituto Nazionale di Ottica - Sezione di Pisa and INFN, Sezione di Pisa*

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Laser-plasma acceleration with self-injection is now established in the laboratory as an "all optical" way to generate relativistic electrons with high energy and high charge per bunch. One route of research is aiming at record values of energy and energy spread for the ultimate outstanding goal of driving an all-optical X-ray FEL. In the mean time, interest for this class of high energy electron sources is growing rapidly for applications in other fields, including biology and medicine and material sciences. For these studies, electron bunches with high charge and relatively stable energy spectra are needed in a simple configuration, likely to be implemented in an application-driven scenario. Several parameters have been considered so far in the experimental investigation of self-injection, including laser and target parameters. However, very little results have been reported on the role of laser polarization, either linear or circular, on the propagation of intense laser pulses in gases and on the subsequent phases of injection and acceleration.

We have carried out a detailed investigation on the role of a range of experimental parameters, including laser polarization, with the aim of identifying key controlling parameters for the generation of high charge electron bunches with energy required for such applications. The experiments were carried out at INO-CNR using the femtosecond laser installation at the Intense Laser Irradiation laboratory. In the experiments, Thomson scattering of laser radiation by plasma electrons is used to measure and optimize the acceleration length while performing energy, divergence and charge measurements on the accelerated electrons. Dosimetry and preliminary radiobiology data will also be presented providing the first indication of effectiveness of this class of sources in view of future clinical studies.

**#181 - Plasmonics**

*Carlo Forestiere (I) - Università degli Studi di Napoli Federico II*

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Plasma Science and Plasmonics are linked by very similar physics: the former deals with electrified gases in which atoms are dissociated in positive ions and electrons, the latter studies the interaction between *free electrons* and the *ion lattice* in a conducting or semiconducting solid. Like gases confining systems are needed to control the shape and volume of plasmas, instead in solids free electrons are naturally confined in the ion lattice region. In both the fields the electromagnetic interaction is the principal protagonist. In particular, the collective electron oscillations upon the excitation by the electromagnetic field are the very central common characteristic. This led to Pines to coin the term *plasmon* to indicate the *oscillations of free electrons in metals* in 1956.

Plasmons play a large role in the optical properties of metals. In particular, the shape of metallic particles determine the plasmons that can be excited resonantly by electromagnetic radiation, which in turn determine the scattered radiation by the particle surface itself. While this mechanism is at the basis of the dichroic Roman glass of the Lycurgus Cup (4th century AD) and the stained glass windows that adorn medieval cathedrals, an understanding of what plasmons are and how they work was not truly established until the 20th century. Seminal works including Lord Rayleigh's theory of light scattering from small particles (1871), Drude's theory of electrical conduction in metals (1900), Maxwell Garnett's theory of light scattering from metal doped glasses (1904) and Mie's theory of light scattering from spherical particles (1908) have explained the coloration of these historical artifacts and are at the basis of plasmonics. On the other hand, Crookes did the first experimental studies of the *fourth state of the matter* in 1879, Langmuir coined the word *plasma* in 1928 and Langmuir and Tonks observed the *electron plasma oscillations* in 1929. Both fields existed separately until 1956 and 1957, first through the work of Pines and then Ritchie, who defined *plasmon* and *surface plasmon*, respectively. In 1970 Kreibig and Zacharias described the optical properties of metal nanoparticles in terms of *localized surface plasmons* and in 1974 Cunningham and his colleagues introduced the term *surface plasmon-polariton* for *propagating surface plasmons*.

Localized surface plasmons allow breaking the diffraction limit for the localization of light into subwavelength dimensions enabling confining and strong field enhancements, which are of particular interest for sensing. Strong field enhancement also enables nonlinear optical effects in structures with metal inclusions. Surface plasmon polaritons are at the basis of ultrafast acousto-magneto-plasmonics for active plasmonic devices and new metrologies. Carbon nanotube and graphene plasmons are emerging as a practicable tool for fast electrical manipulation of light.

### #182 - Fluctuations in plasmas

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Fluctuation theory describes fundamental plasma processes and also provides expressions for the spectral densities of fluctuating plasma quantities as function of the averaged distribution function. This particular outcome of the fluctuation framework constitutes the basis of a number of independent diagnostics that can be implemented in diverse plasma environments. While fluctuation theory is rigorous for collisionless fully ionized plasmas, there exist regimes where approximate methods have to be invoked. Here we discuss our activity on laboratory and numerical experiments exploring such regimes which are intractable by the analytical approach.

For experimental tests of fluctuation theory in ideal plasmas and plasmas seeded with dust, the target environment would be that of a stable quiescent plasma. In most laboratory plasmas the homogeneous state of the positive column is often unstable. Rare exceptions are the so-called brush cathode discharges, where the only fluctuations present are those associated with the thermal motion of the particles. Such a device, the Bari Brush Electrode (BABE), has recently been built by the KTH Complex Plasma Group in collaboration with CNR-Bari (Italy) and unprecedented low fluctuation levels of  $dn/n \leq 10^{-5}$  in He and  $dn/n \leq 5 \times 10^{-6}$  in Ar have been achieved. The discharge also constitutes an appropriate environment for both incoherent and coherent scattering measurements aiming to detect spectral modification due to dust component.

Concerning numerical approach, we utilize molecular dynamics simulations to test the validity domain of theoretical results for the spectral density of plasma density fluctuations in both unmagnetized and magnetized plasmas. We take advantage of a technique based on the analysis of density correlations successfully applied to neutral atomic gases. The method provides a possibility to check model predictions for the spectral densities of plasma fluctuations not only in ideal plasma but also in the presence of neutrals as well as dust particles. This is important for realistic plasma environments where modifications in the spectra due to the presence of solid grains have been proposed as a dust diagnostic in the laboratory and space plasmas.

### #183 - Plasma for Space Propulsion

*Francesco Taccogna - CNR*

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One of the most interesting and full of prospects application in plasma physics are the new type of electric thrusters that will push future space missions into unexplored areas of the solar system or that will allow to enhance the operating lifetime of commercial satellites.

In fact, such devices are characterized by an excellent efficiency, defined as the ratio between the acceleration generated and the mass of propellant expelled. This property is guaranteed by a mechanism of generation and acceleration of ions of noble gases through an ExB configuration inside the thruster channel (also known as Hall effect thruster or closed electron drift derives).

Nevertheless, to date among the main reasons that prevent the use of such devices on a large scale, there is the limited knowledge of the physical processes in the acceleration channel and in particular the so-called anomalous transport of electrons.

The proposed strategy to improve the knowledge is to develop a numerical model based on a three-dimensional full kinetic description (Particle-in-Cell). This technique allows a realistic representation of secondary electron emission from the lateral walls and the electron cyclotron drift instability, phenomena leading to the azimuthal modulation of the plasma parameters in the channel and at the end to the anomalous transport of electrons.

### #184 - Measuring and increasing the safety margins of high-gain shock-ignited targets

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In laser driven fusion a hollow spherical target (containing a layer of DT fuel) is imploded at high velocity by the laser-generated ablative pressure. The goal is to compress the fuel and create a central hot spot, triggering a fusion burn wave. The required laser energy and power decrease strongly as the implosion velocity increases. However, the higher the implosion velocity the higher the

risks associated with Rayleigh-Taylor instability (RTI). The results of the recent National Ignition Campaign (NIC) at Lawrence Livermore Laboratory (LLNL) indeed confirm the difficulty of achieving stable implosions at the velocity required for conventional ignition schemes [1]. In addition, NIC indicates that target designs have to include large safety factors, to account for modelling uncertainties and deviation of target/laser parameters from nominal values.

The shock-ignition (SI) [2] scheme aims at reducing the risks related to RTI by decreasing somewhat the implosion velocity. The hot spot is then created at the end of the implosion by a converging shock driven by a final “spike” of the laser pulse. Significant research activity in modeling and experiments has been devoted worldwide to assessing the feasibility of Shock Ignition [3].

We have studied several aspects of shock ignition by means of analytical models and 1D and 2D numerical simulations with the goal of designing robust targets, also taking into account “lessons” learnt from the NIC. In shock ignition, the separation of fuel compression and ignition allows some design flexibility. We have then determined analytical scaling laws for different scaling options, and have developed a metric to evaluate target ignition margins (or safety factors) [4]. We have then generated gain curves with different safety factors, by means of 1D simulations. The robustness of the design has been then evaluated using 2D hydrodynamic simulations coupled to 3D laser energy deposition. 2D simulations confirm the greater robustness of targets with greater safety factor.

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### #185 - Stimulated Raman Scattering and Two Plasmon Decay instabilities in laser-plasma interaction regime relevant to shock ignition.

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The extent of parametric instabilities at laser intensities  $(3-30) \cdot 10^{15} \text{ W cm}^{-2}$ , relevant for shock ignition approach to Inertial Confinement Fusion, has been investigated at the PALS facility with both calorimetric and spectroscopic tools. Experimental data show that the scattered light is dominated by Stimulated Brillouin Scattering/laser reflection from the critical surface and is larger than ~20%. While the Two Plasmon Decay instability prevails at a quarter-critical density, both Backward Raman Scattering and Forward Raman Scattering are observed at lower plasma densities. The overall energy backscattered by Stimulated Raman Scattering falls by an order of magnitude when random phase plate is used, from 0.3-3% to 0.03-0.12%, depending on density scalelength. The comparison of spectra obtained with and w/o a random phase plate shows that small-scale filamentation and hot spot self-focussing are a determining factor in laser-corona interaction. In particular the use of a random phase plate results in the suppression of Forward Raman Scattering and in a moderate reduction of Backward Raman Scattering. The results suggest that the energy delivery in real SI conditions is limited by SRS rather than by SRS or TPD, which maintain at a low level of reflection and show a saturation at longer scalelengths. However, the investigation of laser-plasma coupling in conditions of longer density scalelengths and higher electron temperature, where growth of instabilities and saturation processes can be different due to the stronger kinetic effects, becomes crucial.

**#186 - Controlling single-spin effects in heterostructured nanowires**

*Stefano Roddaro (I) - NEST, Istituto Nanoscienze CNR and Scuola Normale Superiore*

The control of the orbital and spin state of single electrons in nanostructures is a key ingredient for quantum information processing, novel detector architectures and is more generally of great relevance to spintronics. Coulomb and spin blockade (SB) in double quantum dots (DQDs) enable advanced single-spin operations that could be available even for room-temperature applications in sufficiently small devices. In my presentation, I shall discuss how electrostatic gating can be used to manipulate the spin and orbital quantum state of electrons trapped in a nanowire heterostructure [1,2]. In particular, I shall discuss how it is possible to independently address the charging configuration of two dots separated by only few nanometers by exploiting a differential Stark effect [3]. The method does not require any finely-aligned nanometer gates and thus provides a scalable architecture for the full control of a DQD device, regardless its physical size. In the present implementation, I shall show InAs/InP nanowire DQDs displaying SB beyond 10 Kelvin and a non-monothonic SB suppression in magnetic field.

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**#187 - Brining Spins into Semiconductors**

*Andreas Fuhrer (I) - IBM Research - Zurich*

Spins in semiconductors are thought to be a valuable resource both in potential low-power switching devices and in solid-state quantum computers where the quantum state of an individual spin is used as a qubit.<sup>1</sup> In the first case, device efficiency is usually limited by the quality of spin filters, which polarize a spin current injected into a semiconductor channel. In the second case the challenge lies in controlling and coupling individual spins at the quantum level which poses atomic scale material and fabrication challenges. I will first present non-local spin transport experiments where a ferromagnetic metal is used for injection of spins into GaAs through a Schottky barrier and discuss the influence of ferromagnetic material (Fe/Co), metal-semiconductor interface, hyperfine coupling and spin decay in the semiconductor on a non-local voltage that measures the spin polarization in the semiconductor.<sup>2-4</sup> In a second part I will discuss our efforts to control magnetic impurities in group IV semiconductors at the atomic scale using either self-assembly or scanning tunneling microscope enabled hydrogen resist lithography for placing dopants and magnetic impurities at the atomic scale.<sup>5-7</sup>

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**#188 - Graphene based devices for molecular spintronics**

*Andrea Candini (I) - Istituto Nanoscienze - CNR*

We present our approach to molecular spintronics with graphene. The key idea is to realize novel spintronic nano-devices where the electrical current is controlled by the quantum properties of few single-molecule magnets (SMM) grafted on top of the graphene layer. SMMs are ideal building blocks to develop spintronic devices at the molecular scale. Their advantages with respect to other individual spins in solid state systems include the possibility to chemically engineer with atomic control the intrinsic properties of the magnetic core and the surrounding protecting environment. Thanks to the special combination of low dimensionality and electrical properties, graphene is a natural platform to fully exploit the SMMs functionalities and integrate them in scalable device architectures. In this emerging field, few basic results have already been demonstrated, including the realization of a graphene-SMM nanodevices where the electrical current is sensitive to the molecule magnetization reversal, with sensitivity down to the single molecule level.

Here we will report our most recent advances, exploring two main directions. Firstly, we investigate by means of x-ray absorption the magnetic coupling between single molecule magnets and their environment, including magnetic substrates and graphene. Secondly, we develop graphene based electrodes with gaps in the nanometers range which we employ to graft magnetic molecules in a molecular transistor geometry or to contact atomically precise graphene nanoribbon, which represent the ultimate miniaturization of graphene devices with controllable edges properties and functionalities.

**#189 - Anomalous Friedel oscillations in a quasi-helical quantum dot**

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The charge and spin patterns of a quantum dot embedded into a spin-orbit coupled quantum wire subject to a magnetic field display interesting and unusual properties. Employing a Luttinger liquid theory taking into account open boundaries and finite magnetic field. In the quasi-helical regime, when spin-orbit effects dominate over the Zeeman interaction, we show that peculiar states develop at the Fermi surface of the dot. Anomalous Friedel oscillations with twice the expected wavelength develop in the wavefunction of collective excitations, accompanied by peculiar spin patterns in their magnetization. Both effects are evident in the wavefunction and magnetization of such states, which is analyzed in detail and shown possible to be probed in transport experiments. The stability against electron interactions and magnetic field is investigated. We also discuss how signatures of such states survive in the total charge and spin densities.

#### #190 - Quantization effects and spin-orbit coupling in d-derived states of noble metals

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We study the band structure of thin Au(111) film by a joint ARPES/DFT study with a focus on the deeply lying *d*-derived states. We find an excellent agreement between the experiment and theory, and propose a way to get information about the bulk band structure by examining the two-dimensional quantum well states of thin films. Furthermore we discover a couple of Rashba spin-split surface states, which reside in a deep gap at the *M* point. Comparing to the widely studied *sp*-derived surface states, observed at the  $\bar{\Gamma}$  point of (111) face of the noble metals, these *M*-bar point states have much larger splitting and peculiar properties, such as a strong anisotropy and rhombic warping. A comparative study of Ag(111) film reveals the presence of corresponding surface states, with similar properties and spin-splitting size. This result is unexpected from the point of view of conventional models, developed for the free-electron-like *sp*-derived states, where the amplitude of the splitting depends on the atomic number of the element. Our findings demonstrate the fundamental difference of spin-orbit effects in the *d*-derived states with respect to the *sp*-derived bands.

#### #191 - Spin-polarized surface bands on single layer Bi on Ge(111)

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The spin transport and dynamics in heavy metals with large spin-orbit interaction lies at the cutting edge of spintronics. In particular, large Rashba splittings due to the structural inversion asymmetry have been revealed in single layer heavy metals grown at the top of semiconductor surfaces with the  $C_{3v}$  symmetry [1,2,3], thus enabling the capability to have spin-polarized electron surface bands without the application of magnetic fields. In this context, we have grown a single layer (1 ML) of Bi at room temperature on the top of the n-doped Ge(111) surface and we have studied the interface of this system from a structural and electronic point of view. We have characterized the Bi/Ge interface through low energy electron diffraction (LEED) measurements, revealing the  $C_{3v}$  symmetry which Bi adatoms undergo on Ge(111) and we have mapped the dispersion of the surface bands at low temperature by means of angle- and spin-resolved ultraviolet photoemission spectroscopy (UPS) [4]. We have detected a very large Rashba splitting ( $\alpha_R \approx 1.3$  eV Å) around the *M* point of the Bi surface Brillouin zone, which has been confirmed by spin-resolved measurements, which indicate that these electronic states are almost completely spin-polarized. Notably the Rashba parameter, which governs the removal of the spin degeneracy around the *M* point of the Bi Brillouin zone, is greatly enhanced with respect to the one which is found on the Bi(111) surface, thus evidencing that the spin-orbit coupling of the heavy metals can be strongly increased by the symmetry of the semiconductor surface.

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#### #192 - Femtosecond Time and Angle Resolved Photoemission on Bi<sub>2</sub>Te<sub>3-x</sub>Se<sub>x</sub> Topological Insulators

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Three-dimensional (3D) topological insulators (TIs), a recently-discovered state of matter with unusual surface properties have received special attention during the past few years. TIs are characterized by their spin-momentum locked topological surface states (TSSs) which are conductor despite an energy band gap in the bulk. TSSs have linear dispersion relation as relativistic Dirac fermions, and are protected by back-scattering processes. Owing to these unique features, TIs are presumed to have several applications in the spintronic and quantum computing devices.

Using Time and Angle Resolved Photoemission Spectroscopy (trARPES) by means of pump and probe technique we investigated the real-time energy-momentum map of  $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$  ( $0 \leq x \leq 3$ ) TIs family after excitation of the system by an intense optical pulse in the time domain down to a few tens of femtosecond regime. Furthermore, to study the total angular momenta of the electronic states we exploited circular dichroism (CD) that revealed additional information about the nontrivial surface states of TIs and the temporal evolution of the spin-order in the unoccupied energy bands above the Fermi level. In tr-ARPES study, by reversing the helicity of either circular-polarized “pump” or “probe” beams, we obtained distinct dichroic signals which allowed us to interpret the ultrafast relaxation of carriers in greater detail.

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**#193 - Optical intracellular nanosensing***Francesco Baldini (I) - IFAC-CNR**Other Authors: Barbara Adinolfi, Ambra Giannetti, Sara Tombelli, Cosimo Trono IFAC-CNR Sesto Fiorentino (Firenze)*

Optical sensing exhibited an important role in medicine since the nineties mainly thanks to the invasive capabilities of the optical fibres which allowed unique performances, with measurements inside the human body otherwise impracticable. In the last years, optics enlarged its importance in biomedical area thanks to the advent of nanophotonics which has opened completely new perspectives. Nanoparticles have been shown capable to penetrate the cellular membranes and enter the nucleus of the cell. Their utilisation to deliver sensing molecules inside the cells is one of the new frontiers in nanophotonics applied to biomedicine, although their biocompatibility is still under debate. By proper functionalisation and conjugation of suitable chemical transducers or biological recognition elements, these nanocarriers can deliver sensing nanoprobe for a large variety of chemical and biochemical parameters inside cells. A particular and very challenging class of nanoprobe is given by those where the sensing element is constituted by oligonucleotide optical switches, which are capable to exert therapeutic effects. The nanosensing probe becomes a theranostic agent and the "nanodevice" can work as nanosensor and drug at the same time, by addressing specific RNA messengers and preventing the overexpression of proteins associated to pathologic conditions; in this case nanosensing and drug activity walks side-by-side, being the optical signal associated to the efficiency of the drug. Oligonucleotide optical switches are suitable molecules capable of turning on or modifying their light emission on molecular interaction with well-defined molecular targets. Among these types of antisense oligonucleotide, molecular beacons (MBs) are very promising tools to optically monitor their interaction with the target molecule. In the present presentation, particular attention will be given to the design, implementation and characterization of complex nanostructures for intracellular survivin mRNA monitoring constituted by a molecular beacon, adsorbed on polymethylmethacrylate (PMMA) fluorescent nanoparticles (NPs). The mRNA specific for survivin has been chosen as target, being survivin a multifunctional protein that plays a role in cancer development and progression and highly overexpressed in cancer cells.

**#194 - Nanostructured Sensing Layers for Chemiluminescence Biosensing***Loic J. Blum (I) - Lyon 1 University / CNRS**Other Authors: Christophe A. MARQUETTE*

The key element in the design of sensor and biosensors is the sensing layer which to a great extent gives the specificity/selectivity and the sensitivity to these sophisticated tools.

Because of its great sensitivity, the luminol chemiluminescence (CL) reaction catalyzed by horseradish peroxidase I the presence of hydrogen peroxide is often used as the detection system for biosensors and biochips. The light emission can be enhanced by chemical compounds such as 4-iodophenol. Beside this luminescence enhancement due to a chemical reactant, a physical approach has been also developed to enhance the light emission of the peroxidase-catalyzed luminol CL. Nano-structuring of the sensing layer can have a dramatic effect through the amplification of the detected signal.

For that purpose, peroxidase was immobilized on biochips at the surface of flat "bulk-like" and rough "cluster-like" metal films at a distance controlled by a peptide chain with a length between 1.3 and 7.8 nm. When the CL of the luminol/H<sub>2</sub>O<sub>2</sub> system is catalyzed by peroxidase in the presence of a metal-corrugated film, a strong CL enhancement is observed. The magnitude of enhancement depends on different factors such as the morphology of the thin metal film, the nature of the metal, the pH value of the reaction medium as well as the distance between peroxidase and the surface. Exploiting this enhancement phenomenon, DNA chips and immunochips have been designed using nano-structured gold-modified carbon microarrays and it was observed the chemiluminescent signal was over a hundred times and two hundred times more intense, respectively than with a standard carbon surface.

**#195 - Bulk and Hollow Whispering Gallery Mode Microcavity - based Immunoassay***Simone Berneschi - IFAC-CNR**Other Authors: Francesco Baldini (IFAC-CNR), Andrea Barucci (IFAC-CNR), Alessandro Cosci (Centro Studi e Ricerche "Enrico Fermi" & IFAC-CNR), Franco Cosi (IFAC-CNR), Daniele Farnesi (Centro Studi e Ricerche "Enrico Fermi" & IFAC-CNR), Gualtiero Nunzi Conti (IFAC-CNR & Centro Studi e Ricerche "Enrico Fermi"), Giancarlo C. Righini (Centro Studi e Ricerche "Enrico Fermi" & IFAC-CNR), Silvia Soria (IFAC-CNR), Sara Tombelli (IFAC-CNR), Cosimo Trono (IFAC-CNR), Stefano Pelli (IFAC-CNR & Centro Studi e Ricerche "Enrico Fermi"), Ambra Giannetti (IFAC-CNR)*

Whispering Gallery Mode (WGM) resonators in the bulk and hollow core geometries, such as optical silica microsphere and microbubble, due to their high Q factors ( $> 10^7$ ), small mode volumes and long storage lifetime for the trapped photon inside the cavity, guarantee a high light – matter interaction. These features make them a promising optical platform for the development of highly performant bio-sensors. Their working principle is based on the morphological WGM dependence: any change in the external surface of the microsphere or in the inner wall of a microbubble, due to some chemical and/or biochemical bonding, causes a shift of the resonances and reduces the Q factor value of these microcavities. By measuring this shift, it is possible to

obtain important information about the concentration of the analyte to be detected. We fabricate these WGM resonators by an arc discharge process which involves a tip of an optical single mode fiber and a pressurized silica capillary. In the former case, due to the superficial tension, the partially fused fiber tip assumes a spherical shape during the following cooling step; in the latter, due to the pressure inside the microcapillary, the microtube increases its radial size until to reach a spherical bulge shape (the so called microbubble) locally in correspondence of the heated region of the same microcapillary. The resonances excitation in these microstructures occurs by evanescent field tail coming from a guiding structure (i.e.: a tapered fiber or a channel waveguide). A crucial step for the development of a WGM based biosensor is constituted by the functionalization of its surface. This process should guarantee a good uniformity and homogeneity for the so deposited bio-layer in order to preserve high Q factor ( $> 10^5$ ) for the optical transducer even in phosphate buffered saline (PBS). Here we report on the development of an *ad-hoc* chemical procedure able to satisfy the aforementioned requirement. In particular, for the hollow core WGM microbubble resonator, we adopt a spatially selective photo-chemical process able to selectively bond the bioreceptor only in correspondence of the microbubble inner wall. We demonstrate the feasibility of these methods by an IgG/anti-IgG reaction, with the anti-IgG which is fluorescently labeled. The bulk and hollow WGM microcavities capability of working as an immunoassay platform is proved by different optical techniques, such as real time resonance shift and broadening and fluorescence microscopy.

### #196 - LAB-ON-A-CHIP MICROFLUIDIC IMAGING BY EXTENDED FIELD OF VIEW DIGITAL HOLOGRAPHY

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The study of biological specimens onboard Lab-on-a-Chip (LoC) platforms is well assessed and raises growing interest for point-of-care diagnostics. In this framework, great effort has been spent to develop compact chips with embedded imaging functionalities. Label-free techniques are preferred for non-invasive ex-vivo inspection of the samples. Among them, Phase shift Interferometry (PSI) and Digital Holography (DH) have been proved to yield quantitative phase-contrast mapping as well as flexible numerical refocusing. In PSI a phase shift between multiple interferograms has to be provided, e.g. by piezoelectric actuators, to synthesize the whole complex object field. Here we show an interesting imaging modality, named Space-Time Scanning Interferometry (STSI), which exploits a lateral displacement between the object and the detector, provided by a translational stage, to synthesize a new space-time interferogram with interesting features. Indeed, a single linear sensor array is sufficient to build up a synthetic interferogram with unlimited Field of View (FoV) along the scanning direction and improved Signal-to-Noise Ratio (SNR). Besides, if a small subset of lines of the detector are selected, synthetic interferograms can be obtained, shifted each other of the desired phase step for phase retrieval purposes. The theoretical formulation and experimental proofs of the STSI method applied to different and complex shaped pure-phase objects (e.g. polymeric drops) are reported. PSI is applied to properly shifted synthetic interferograms (PS-STSI) to demonstrate the capability of estimating the whole complex object field. Noteworthy, the STSI principle is well-suited to be adopted in all the cases where the object motion is an intrinsic feature of the system, such as in case of microfluidics, so that the advantages of STSI have no cost associated with. Starting from these considerations, we discuss the application of the STSI method to in-flow on-chip microscopy. By performing out-of-focus recordings with a single line detector, a Space-Time Digital Hologram (STDH) could be synthesized carrying full-field information of the flowing samples. A so built STDH still maintains all the advantageous capabilities of DH microscopy, i.e. quantitative phase-contrast mapping and flexible numerical refocusing. Moreover, a re-focusable STDH with unlimited FoV along the flow direction can be created adopting a single linear detector and with no need for hologram stitching. Promising first-cut results, obtained using polystyrene beads as test samples, will be reported. Hence, it could be possible to move a step toward the integration of the imaging functionalities onboard chip for high-throughput rapid diagnostics.

### #197 - CNT-based devices for biosensing applications

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In this work carbon nanotubes (CNTs) - based devices were produced for biosensing applications. Dielectrophoresis (DEP) has been used to accurately control the deposition of multi-walled CNTs between electrodes. This technique is a low cost and room temperature deposition method that can be used on different substrates (silicon, glass, plastics) for large scale production of chemical or biological sensors. The devices have been tested for the detection of proteins, such as arginase and lysozyme, after suitable functionalization of CNTs with specific antibodies. Scanning electrical microscope (SEM) and electrical characterization

have been performed on the biosensors before and after protein exposure. Sensitivity, specificity and stability of the sensing devices have been evaluated.

### #198 - Silicon photomultipliers as transducers for DNA hybridization detection

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Optical transduction is the most used method to recognize DNA hybridization with traditional markers used in commercial systems. In DNA microarrays, a nucleic acid (target) labelled with a fluorescent molecule (e.g. with CY5) hybridizes with the complementary sequences contained in the probes anchored onto a surface [1]. In Real Time Polymerase Chain Reaction (RT-PCR) the fluorescence of Fluorescein (FAM) increases during the DNA amplification. In both systems, a scanner detects the fluorescence signal, and an image analyser software elaborates the images to quantify the signal.

Aim of our work is to replace the traditional detection system, in both RT-PCR and DNA microarray applications, with an optical sensor based on a pixel array of solid state detectors (Silicon Photomultipliers, SiPM), produced by STMICROELECTRONICS in Catania. Each pixel is formed by the series between a single photon avalanche diode, operating in Geiger mode, and a quenching resistor. All pixels are connected in parallel to a common load where the output signal is collected [2].

A 25 pixels SiPM was electro-optically characterized. This device can compete in sensitivity with traditional photomultiplier tubes achieving low power consumption, small physical size and insensitivity to magnetic fields.

To measure the fluorescence emitted by biological molecules we used an experimental set up based on a fiber-coupled laser hitting orthogonally on the sample. The sensor is placed at 45° with respect to the normal axis to the sample; between the sensor and the sample is interposed a bandpass filter, centered at the fluorophore emission wavelength to suppress the laser radiation reflected by the support. The signal is acquired using a home-made software developed in Labview®, and, then, processed with Matlab®.

To determine the sensor detection limit, FAM measurements in liquid (10µl) and CY5 spotted on solid surfaces, both at molar concentrations ranging from 100 fM to 5nM, were performed. We found that the sensor response is linear over the measured range. This result underlines the SiPM higher sensitivity with respect to commercial optical system in detecting very low fluorescence signals. The SiPM properties and the system potentialities allow their miniaturization, opening up the possibility for the design and fabrication of a cheap, easy and portable optical systems.

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### #199 - Uptake of Silica covered Quantum Dots on living cells: long term vitality and morphology study on Hyaluronic acid biomaterials

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Quantum Dots (QDs) are crystalline semiconductor nanoparticles which show unmatched optical features with bright photon emission. After the UV-visible optical absorption the so acquired exciton energy is mainly relaxed by emitting a fluorescence photon typical in the visible region. The key of the enormous growth of research studies on QDs relies on the quantum confinement effect, which is due to comparable nanometric scale of both the Bohr exciton radius and the geometrical confining dimension of the system. This explains the precise control which is obtained on the discrete exciton energy levels and thus on the wavelength of fluorescence peak, ranging between UV and IR regions as a function of dimension and relative excitons quantum confinement. In the last years, the direct colloidal synthesis of QDs guarantees the formation of highly mono-disperse nanoparticles with well controlled optical features. These systems show also a very high brightness and resistance to photo-damage under continuous illumination, in respect to conventional organic dyes. This aspect is crucial to utilize QDs as biophysical probes but some problems should be overcome: i) most of QDs are prepared using some toxic atoms, ii) the fluorescence of QDs is really sensible to the external environment because of the presence of electronic traps on their crystalline surface could act as fluorescence quenchers or to give rise to strong emission instability. One way to overcome this drawbacks is to create a protective shield around the dot in order to avoid both external fluorescence quenchers and to block any contact of toxic atoms with the external biological environment.

In this work we prepared colloidal CdSe-CdS core-shell nanocrystal emitting @625 nm and, by a micro-emulsion procedure of water in oil inverse micelle, we encapsulated a single dot inside each silica sphere. In this way the nanoparticles became biocompatible, are simply to prepare and could be used also in a water based environment. Moreover, the silica shield is transparent to the

wavelengths of interest. Here we demonstrate that it is possible to employ this silica-QDs as a stable and non-toxic fluorescent probe for cell staining with the aim to use these fluorescent cells as a means of characterization of biomaterials of different nature. In particular, since it is well known that RGD peptide is a recognition sequence for integrins that strongly increase the tendency of the cells to adhere onto various surfaces, we produced a derivative of hyaluronic acid functionalized with different

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**#200 - RIXS as a probe of spin-orbit Mott insulating iridates**

Marco Moretti (I) - ESRF - The European Synchrotron

Spin-orbit coupling is the main ingredient for 5d transition metal oxides to form novel electronic states of matter, such as the recently discovered Mott insulating state in  $\text{Sr}_2\text{IrO}_4$  [1-3]. This insulating behavior is unexpected in iridate perovskites because, for a half-filled shell with spatially extended orbitals, electronic correlation was thought to be negligible. Instead, the role of electronic correlation is enhanced here by spin-orbit coupling through the formation of the so-called  $j_{\text{eff}} = 1/2$  ground state. Its realization arises from the interaction of strong spin-orbit coupling and cubic crystal field, and is perturbed by short- and long-ranged anisotropies which could cause departures from the  $j_{\text{eff}} = 1/2$  ground state. In my talk I will show how resonant inelastic x-ray scattering (RIXS) can be used to probe the ground state of iridates and gain insight into their electronic ground and excited states.

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**#201 - SPIN DEGREES OF FREEDOM IN RELATIVISTIC FERROELECTRICS**

Silvia Picozzi (I) - Consiglio Nazionale delle Ricerche (CNR-SPIN) L'Aquila

Other Authors: Domenico Di Sante (CNR-SPIN, L'Aquila), Alessandro Stroppa (CNR-SPIN, L'Aquila), Paolo Barone (CNR-SPIN, L'Aquila)

By exploiting the interplay between spin and dipolar degrees of freedom via spin-orbit coupling in ferroelectric semiconductors, I will focus on the tight link between k-dependent spin-splitting in the electronic structure, spin-texture and electric polarization. Based on density functional simulations, I will show our theoretical predictions of a giant Rashba spin-splitting in "bulk" GeTe[1], prototype of novel multifunctional materials - labeled as Ferro-Electric Rashba Semi-Conductors (FERSC)[2] - where the chirality of the spin texture is one-to-one linked to polarization. As the latter can be induced/controlled/switched via an electric field in a non-volatile way, the integration of semiconductor spintronics with ferroelectricity is envisaged. In the last part of the talk, the connection between ferroelectricity and spin-degrees of freedom will be discussed by providing examples from different materials classes (oxides heterostructures, halides perovskites,[3] chalcogenides,[4] etc), all of them showing strong relativistic effects.

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**#202 - Exploring the scientific opportunities of resonant inelastic soft x-ray scattering with the new ERIXS instrument at the ID32 beamline of the ESRF**

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In the last few years, soft resonant inelastic x-ray scattering (RIXS) has led to enlightening results in the study of strongly correlated electron systems, and in particular high- $T_c$  superconducting cuprates. AXES and SAXES [1] spectrometers, working in the soft x-ray range (400 - 1500 eV) at the beam lines ID08 of the ESRF (since 1995) and ADDRESS of the Swiss Light Source (since 2007) respectively, have been proved to be extraordinary tools to study medium- and low-energy excitations in solids and thin films, whose excitation spectra can bring illuminating information on the basic interactions at play, such as magnetic coupling [2-3], chemical bond anisotropy (crystal field), strength (phonons, vibrational modes) and charge ordering [4].

The new ERIXS (European-RIXS) instrument, at the ID32 beamline of the ESRF, offers unprecedented and unique performances for high resolution RIXS, in terms of energy resolution (i.e. allowing to measure with a combine bandwidth decisively better than

anywhere else), diffractometer-quality sample environment, polarization control and high luminosity. In this sense, it was extremely important to deepen exploit the new features of the facility.

Here we present the scientifically pioneering work done to explore the new scientific opportunities offered by ERIXS, by performing several experiments serving as first demonstration of new classes of research. We will show results coming from the advanced commissioning of the instrument at several photon energies for realistic experimental conditions and scientifically interesting samples.

We mainly worked at Cu- $L_3$  edge, on high- $T_c$  superconducting cuprates, well known to offer a wealth of interesting scientific problems to be studied with RIXS. We also tuned the energy at other edges (O-K edge, Mn- and Ni- $L_3$ , Gd- $M_5$ ), both to characterize the instrument and to explore new scientific opportunities in other systems, allowing to extend the technique to the study and the characterization of a wide class of correlated systems.

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### #203 - Spin-orbital physics in hybrid 3d-4d oxides

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The entanglement of spin, orbital and lattice degrees of freedom in correlated systems is known to lead to intricate quantum phenomena [1-3], including exotic quantum topological states [4]. Correlated physics in transition metal oxides (TMO) traditionally emphasizes 3d materials because the more extended 4d-shells would a priori suggest a weaker ratio between the intra-atomic Coulomb interaction and the electron bandwidth. Nevertheless, the extension of the 4d-shells points towards a strong coupling between the 4d-orbitals and the neighboring oxygen orbitals, implying that these TMO have the tendency to form distorted structure with respect to the ideal one. Hence, the change in M-O-M bond angle often leads to a narrowing of the d-bandwidth, bringing the system on the verge of a metal-insulator transition or into an insulating state. The interplay between more localized 3d and more delocalized 4d states tunes the competition between correlated metallic and Mott-insulating states and, in turn, can significantly influence the strength and the hierarchy between the spin-orbital-lattice degrees of freedom. In this framework, we study how the magnetic and orbital patterns in a uniform 4d host are modified by the inclusion of 3d impurities substituting the 4d ions. After discussing the most suitable microscopic models for different types of 3d-4d hybrids, we determine the phase diagram assuming different conditions for the orderings, both for metallic [5] and insulating cases [6]. We demonstrate that the coupling between the impurity and the host, specific of the 3d-4d elements, can generate a complex phase competition [5-6]. Since ruthenates belonging to the Ruddlesden-Popper series represent a fertile 4d platform where to achieve different magnetic-orbital ordered states and metal-to-insulator transitions [7-9], a specific discussion of the Ru-oxides doped with Mn will be presented.

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### #204 - Dynamical properties of hybrid perovskites at finite temperature investigated by large-scale model potential molecular dynamics

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The success of hybrid lead halide perovskites in photovoltaics has given rise to an intense research effort to study its fundamental properties and the role of the organic and inorganic components in the hybrid material. The electronic levels of the molecules are not directly involved in the optoelectronic processes and the intrinsic recombination and photovoltaic properties correspond to that of an inorganic semiconductor with a hybrid body [1]. However, the actual molecular orientations have an impact on the distortions of the inorganic lattice and, in turn on the electronic and transport properties [2]. At finite temperature, the interplay between the rotational dynamics of the molecules and the inorganic lattice is important to understand the relaxation processes and the molecular order within the material. Most of the dynamical studies have been performed by first-principles methods ([3]).

However, a comprehensive study of the effect of temperature on the reorientational dynamics requires to extend the time and length scale of atomistic simulations. Here, we report on the development of a simple ionic interatomic model with reduced computational cost and to its application to study dynamical properties of the hybrid perovskites [4]. The model makes possible to study the molecular reorientational times, calculated under controlled thermodynamical conditions, spanning from the orthorhombic to the cubic phase. The results are consistent with experimental data and analyzed by a simple analytical model that clarifies effect of temperature on the relaxation phenomena[4]. Furthermore, the present model potential opens the way to the large-scale atomistic simulations of dynamical processes in hybrid perovskites and its nanostructures. We discuss showcase applications including infrared absorption, point-defects mobility, degradation phenomena in vacuo and in water[5]. References [1] Filippetti, A.; Mattoni, A. Phys. Rev. B 2014, 89, 125203. [2] Filippetti, A.; Delugas, P.; Mattoni, A. J. Phys. Chem. C 2014, 118, 24843. [3] Quarti, C.; Mosconi, E.; De Angelis, F. Chem. Mater. 2014, 26, 6557-6569. [4] Mattoni, M.I. Saba; A; Filippetti A; Delugas P.; 2015 , accepted JPC C [5] Mattoni, M.I. Saba; A; Filippetti A; Delugas P.; in preparation

### #205 - Non-adiabatic effects in transition metal dichalcogenides

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In this talk I will present the effect of the atomic zero-point motion on the bandstructure of transition metal dichalcogenides. The bands show a high sensitivity to the atomic motion which has crucial consequences on the optical properties. I will show the trends for the monolayer, bilayer and bulk materials.

### #206 - Weak Magnetism in Superconducting Thin Films under Electric Field Effect

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Superconductivity and ferromagnetism are usually incompatible phenomena, however they can coexist in high  $T_c$  superconductors single films and in proximity with ferromagnetic manganites. A systematic study of the Cu L<sub>2,3</sub> edge X-ray Magnetic Circular dichroism (XMCD) has shown that the out-of-plane component of the canted Cu<sup>2+</sup> spins aligns parallel to the magnetic field, giving rise to a net magnetization in undoped (La<sub>2</sub>CuO<sub>4</sub> (LCO)), underdoped, and optimally doped La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> (LSCO), NdBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-δ</sub> (NdBCO) and YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-δ</sub> (YBCO) compounds [1]. Recently, we demonstrated that the charge transfer of spin-polarized electrons from La<sub>0.66</sub>Sr<sub>0.33</sub>MnO<sub>3</sub> ferromagnets to La<sub>1.85</sub>Sr<sub>0.15</sub>CuO<sub>4</sub> thin films in (La<sub>0.66</sub>Sr<sub>0.33</sub>MnO<sub>3</sub> / La<sub>1.85</sub>Sr<sub>0.15</sub>CuO<sub>4</sub>) superlattices induces an unusual weak ferromagnetic order in the CuO<sub>2</sub> layers. This unusual magnetic order is associated to the canting of the Cu<sup>2+</sup> magnetic moments and propagates from the interface inside the superconductor via the Dzyaloshinskii-Moriya interaction over distances much larger than the superconducting coherence length. [2]. Here, we report a study of the electronic properties of Nd<sub>1.2</sub>Ba<sub>1.8</sub>Cu<sub>3</sub>O<sub>7+x</sub> thin films as a function of the electric field in devices characterized by a doping nearby the superconducting-insulating (S-I) transition [3]. Cu L<sub>2,3</sub> edge XMCD measurements show that the out-of plane Cu spin moment is tuned by electric field effect. In particular, the doped thin films show a paramagnetic behaviour as a function of the magnetic field, independently from the carrier density tuned by field effect. This reflects the short range antiferromagnetic fluctuation of Cu-spins in the CuO<sub>2</sub> planes. [1] G. M. De Luca, et al. Phys. Rev B 82, 14504 (2010) [2] G.M. De Luca, et al. Nat. Commun. 5:5626 doi: 10.1038/ncomms6626 (2014) [3] M. Salluzzo, et al. Phys Rev Lett. 100, 056810 (2008)



**#207 - Hybrid materials for Photovoltaics and Photovoltachromics**

Giuseppe Gigli (I) - Istituto di Nanotecnologia- CNR NANOTEC

The exploration of innovative materials and device architectures is constantly fostering our solar conversion research activity, aiming at low cost and highly efficient solutions.

From conceptually new mesostructured solar cells, based on self-assembling hybrid perovskites, to full inorganic bulk heterojunction solar cells based on versatile nanocrystals, we have been exploring viable routes for an effective market impact of third generation photovoltaics.

Our vision is based on solution processable materials and low temperature cell manufacturing, matching the requirements of existing technologies, for large-scale device production at reasonable production costs. Furthermore we pursue the implementation of such solar converting components into multifunctional devices, an example we conceived on this line, is a photovoltachromic cells integrating both photovoltaic and photoelectrochromic functionalities, targeting building integration.

**#208 - A Supramolecular Approach to Artificial Photosynthesis: A Concert for Photons and Electrons**

Sebastiano Campagna (I) - University of Messina

Conversion of solar energy into fuels (artificial photosynthesis) is one of the Holy Grail of Science. Solution of this complex problem is quite appealing, as it could alleviate the huge energy problems which our society is going to face. Artificial photosynthesis, according to a bio-mimetic approach, requires the design of several components, each of them a supramolecular system, structurally organized and functionally integrated. Indeed, in analogy with the natural photosynthetic systems, in such integrated assemblies, photons and electrons have to be elaborated in a well-organized fashion, and all the process must be orchestrated in terms of space, energy, and time.

Here we present some recent results obtained by our group related to (i) artificial light-harvesting antenna systems (their role: absorbing light and converting it into electronic energy, which can be funnelled to specific sites of the assemblies); (ii) charge separation systems (role: to use the electronic energy collected by the antennae to perform charge separation, that is to transform electronic energy into redox energy); (iii) integrated antenna and catalysts for water oxidation.

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**#209 - Newly synthesized organic polymers/amorphous silicon hybrid solar cells: thickness effects**

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Organic solar cells based on semiconducting molecules and macromolecules improved largely during the last few years, breaking the 10 % efficiency barrier [1]. Many of these polymers absorb strongly in the red part of the spectrum, even beyond 750 nm, and can be easily processed from solution. However, most of these devices use soluble fullerene derivatives, which have an only weak absorption in the visible spectral range. Therefore, research has been devoted to alternative acceptor materials. One possibility is the use of inorganic semiconductors. Among these, hydrogenated amorphous silicon is highly promising as it can be processed in thin film photovoltaic devices and it possesses good absorption from blue to green, which is complementary to the absorption of some of the low bandgap polymers used in efficient organic photovoltaic devices. Thus, improved efficiency is expected for hybrid devices, which combine amorphous silicon and organic materials in a single hybrid device [2–4].

Here we present a study on the performance of hybrid solar cells comprising a planar heterojunction between a novel conjugated acceptor polymer and hydrogenated amorphous silicon (a-Si:H).

Hybrid polymer/amorphous silicon cells have a p-i-n structure realized on glass/FTO substrate. The n-type organic polymer was spincoated from different concentration solutions with resulting layer thicknesses approximately ranging from 20 nm to 100 nm. Ag contacts were sputtered on top of the device.

We evaluate the effect of organic layer thickness in the hybrid solar cells. In detail, it is shown that the electrical behavior (I-V characteristics) of the hybrid polymer/silicon solar cells improve when the thickness of the polymer decrease. One reason for this is the intrinsically short diffusion length of excitons in organic semiconductors, which are typically around 10-20nm.[5,6]

Using the poly(2,5-di(3,7-dimethyloctyloxy)cyanoterephthalylidene) commercial product as reference sample, the novel polymer reaches a better photovoltaic performance.

Moreover, we observe a further improvement of the solar cell performance with the use of a molecular connector containing an aza group in trans configuration that determines the formation of a complex supramolecular architecture.

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## #210 - Charge dynamics and interface properties in hybrid halide perovskite-based solar cells

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The recent employment of self-assembling hybrid halide perovskite in solar converting devices has been depicted as the “Next Big Thing in Photovoltaics”.<sup>1</sup> Despite the rapid increase in efficiency associated with the evolution of this technology, and the expanding body of dedicated works, many of the fundamental questions concerning the material properties affecting device operation remain unanswered.<sup>2</sup> In particular, further developments of this technology, require a rationalization of the carriers generation and transport mechanisms for all the diverse device configurations in which perovskite has been embedded. Here we propose a picture for carriers generation and recombination in highly efficient perovskite-based solar cells employing TiO<sub>2</sub>, NiO or Al<sub>2</sub>O<sub>3</sub> as flat or mesoporous substrates and spiro-OMeTAD or PCBM as solid state complementary charge extracting materials. Time Correlated Single Photon Counting, Photoinduced Absorption and Transient PhotoVoltage measurements were selected as direct investigative tools for the determination of such phenomena in model systems and working devices. The collection of our results depicts a peculiar behaviour for charge generation and dynamics, as the presence of two n-type materials, in TiO<sub>2</sub> including devices, generates alternative paths for electron transport. In addition our results suggest that performance in devices with perovskite overlayer is mainly ruled by the overlayer, whereas the mesoporous layer influences the contact properties.<sup>3-6</sup> The important new insights, contained in these works, would help the comprehension of these innovative devices suggesting potential design improvements.

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## #211 - Electric field stress effect and role of electrode material on the improvement of hydrogenated amorphous silicon solar cells

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Hydrogenated amorphous Si (a-Si:H) solar cells are strongly affected by the well known Staebler- Wronski effect occurring during light soaking of a-Si:H photovoltaic cells. Consequence of this is a substantial loss of solar cell parameters performances and, hence, a worsening of cell power conversion efficiency compared to time zero performance. The Staebler-Wronski effect, taking place in solar cells both under operation and in open circuit condition, is believed not to be an extrinsic effect, but rather a basic phenomenon related to the nature of a-Si:H and to the stability and motion of H-related species in the a-Si:H lattice. In this work we show an electrical method to counteract the above-discussed solar cell ageing effects. In detail, it is shown that the application of a reverse bias stress in presence of illumination not only slows down the solar cell ageing kinetics but even produces an improvement of the cells parameters as a function of stress time, especially of the series resistance, of the open circuit voltage, and of the overall power conversion efficiency. We also show that an analogous improvement (reduction) of sheet resistance is also observed applying a high intensity electric fields in single thin films of doped a-Si:H deposited on SiO<sub>2</sub>. Finally, we demonstrate that

type of bottom contact over which the a-Si:H is grown by PECVD has a strong influence on the recovery-improvement kinetics: SnO:F (FTO) transparent conductive oxide (TCO) and molybdenum bottom contacts to the p-type a-Si:H layer are here compared. These results suggest that the observed improvement of the overall power conversion efficiency in the p-i-n solar cells, and of the sheet resistance in individual p-type a-Si:H films deposited on SiO<sub>2</sub> is due to the motion of light ions from the oxide to the a-Si:H films (or vice-versa) driven mainly by the electric field. \*

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#### #212 - Semi-transparent perovskite photovoltaic and solid-state electrochromic cells

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Photovoltachromic devices combine photovoltaic and electrochromic features to enable adjustable transparency glazing, where the photovoltaic component supplies the power to drive the coloration.

Such stand-alone, self-powered devices are of commercial interest for integration into windows and surfaces of buildings and vehicles. Here, we report for the first time some recent results in the design of liquid junction and solid state perovskite-based photovoltachromic devices, with self-adaptive transparency.

This multifunctional devices are capable of producing electrical power by solar energy conversion as well as undergoing a chromic transition from neutral-color semitransparent to dark blue-tinted when irradiated with solar light, without any additional external bias. Recently, we demonstrated that the combination of semi-transparent perovskite photovoltaic and solid-state electrochromic cells enables fully solid-state photovoltachromic devices with a suitable visible transmittance as well as a 5.5% maximum light power conversion efficiency. These results represent a significant step towards the design of a smart building envelope and the building integration of photovoltaics.

#### #213 - Morphological Tailoring of low-cost ZnO Nanorods for Application in Solar Cells

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Efficient light management is today a key challenge to achieve cost-effective and high efficiency solar cells. The strategies developed for enhancing the light absorption involve the employment of many types of nanostructured materials. In particular, a light diffuser top layer is widely used in thin film technology solar cells for extending the path length of incident light into the absorbing layer. Nonetheless, detrimental drawbacks appear often on the electrical performances. Nanostructured zinc oxide has been shown to be a promising option for effectively scattering the visible and near infrared radiation. It is a nontoxic and abundant material and it can be easily synthesized on different substrates, also by low cost methods [1]. We investigated the forward light scattering properties of transparent ZnO nanorods (120–1300 nm long, 280–60 nm wide) layer synthesized by chemical bath deposition, getting transmission haze as high as 70% at 400 nm wavelength. The shape and size of ZnO nanorods have been varied by changing the molar concentration of the reagents in the growth solution. Scanning Electron Microscopy (SEM) investigations revealed the particular morphologies of ZnO nanostructures prepared using various growth parameters and X-ray diffraction (XRD) measurements have shown a clear texture along [0002], in agreement to expectations. Through a simple light scattering simulation, it was possible to clarify the influence of NRs morphology on the radiation diffusion and estimate a threshold in the NRs length (about 1 μm) over which the light scattering is significantly enhanced. Finally, we applied a light scattering film based on ZnO NRs layer to a thin c-Si solar cell and measured an increase of the external quantum efficiency for wavelengths larger than 600 nm, without any degradation of cell performance. The results suggest that light scattering by ZnO NRs can be successfully applied to solar cell via a simple integration scheme [2]. Further improvement of the NRs size and density will be presented and discussed, also on different solar cell types. References: [1] V. Strano, R. G. Urso, M. Scuderi, K. O. Iwu, F. Simone, E. Ciliberto, C. Spinella, and S. Mirabella, *J. Phys. Chem. C* 118, 28189 (2014). [2] V. Strano, E. Smecca, V. Depauw, C. Trompoukis, A. Alberti, R. Reitano, I. Crupi, I. Gordon, S. Mirabella, *Appl. Phys. Lett.* 106, 013901 (2015).

#### #214 - Molecular-Level Switching of Polymer/Nanocrystal Non-Covalent Interactions and Application in Hybrid Solar Cells

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Hybrid composites obtained upon blending conjugated polymers and colloidal semiconductor nanocrystals are regarded as attractive photoactive materials for optoelectronic applications. Here it is demonstrated that tailoring nanocrystal surface chemistry permits to control non-covalent and electronic interactions between organic and inorganic components. The pending moieties of organic ligands at the nanocrystal surface are shown to not merely confer colloidal stability while hindering charge separation and transport, but drastically impact morphology of hybrid composites during formation from blend solutions. The relevance of this approach to photovoltaic applications is demonstrated for composites based on poly(3-hexylthiophene) and lead sulfide nanocrystals, considered as inadequate until this report, which enable the fabrication of hybrid solar cells displaying a power conversion efficiency that reaches 3%. By investigating (quasi)steady-state and time-resolved photo-induced processes in the nanocomposites and their constituents, it is ascertained that electron transfer occurs at the hybrid interface yielding long-lived separated charge carriers, whereas interfacial hole transfer appears hindered. Here a reliable alternative aiming to gain control over macroscopic optoelectronic properties of polymer/nanocrystal composites by mediating their non-covalent interactions via ligands' pending moieties is provided, thus opening new possibilities towards efficient solution-processed hybrid solar cells.

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**#215 - Perovskite Solar Cells and Modules**

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A new promising class of light harvesting materials, namely the hybrid organic halide based perovskites, have been recently employed to realize high efficiency photovoltaic solar cells. This kind of crystalline material shows broad absorption in the visible spectrum (direct energy gap down to 1.55 eV), good electron and hole conductivity, delivering also high open circuit voltages in photovoltaic devices.

For small area devices, a power conversion efficiency (PCE) of 18.4% has been reached using a bilayer structure consisting of 85% formamidinium lead iodide (FAPbI<sub>3</sub>) and 15% of methylammonium lead bromide (MAPbBr<sub>3</sub>) [1], while the record efficiency has been certified to be 20.1% by the National Renewable Energy Laboratory [2]. Similarly, the development of large active area prototypes [3] has evolved with an equal impressive pace, achieving  $\eta=13%$  [4] on 10 cm<sup>2</sup> and  $\eta=9.6%$  on an even larger active area (100 cm<sup>2</sup>) [5-6].

In this talk, we will present the efforts made to develop Perovskite Solar Cells (PSCs) on small and large area and a simulation study to understand the main physical mechanisms governing the behaviour of PSC. The influence of the Hole Transporting Layer on the device characteristics will be presented together with the use of 2D materials to improve device performances. A detailed analyses on PSCs stability will be presented.

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**#216 - Light trapping and efficiency limits in thin-film silicon solar cells**

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Light trapping is crucial to increase efficiency in thin-film solar cells by approaching the ultimate limit to absorption, which is usually taken to be the Lambertian limit. High-efficiency solar cells have to "optically thick but electronically thin" in order to maximize both optical absorption and carrier collection. These contradictory requirements can be reconciled by implementing advanced light trapping approaches.

In this work [1] we focus on solar cells made of crystalline silicon, which represent the dominant technology in the market. Light trapping at the wavelength-scale can be performed with ordered, disorder, or hybrid photonic structures. We performed a theoretical study of a number of such structures by means of rigorous coupled-wave analysis. In particular, randomly rough surfaces with Gaussian disorder are found to describe well the scattering properties of actual rough substrates, and to approach the Lambertian limit of scattering in a wide range of Si thicknesses.

Moreover, we report on theoretical solutions of the transport problem by means of analytical modelling and by a fully numerical solution of drift-diffusion equations with the finite-element method. The combination of optical and electronic simulations allows to determine the optimal thickness in view of maximizing the energy conversion efficiency. We consider both bulk and surface recombination in solar cells with the absorber thickness ranging from 1 to 100 micron or more. Our results predict that with state-of-the-art material quality of thin c-Si layers, the optimal absorber thickness is of the order of tens of microns or higher. Thin-film solar cells with realistic material parameters can outperform bulk ones, provided surface recombination is below a critical value, which is compatible with present-day surface passivation technologies.

Finally, we explore the efficiency limits in single-junction c-Si solar cells, focusing on the roles of intrinsic (Auger) and extrinsic recombination mechanisms. The limiting efficiency is close to 29%, as compared to the current record of 25.6%. We identify incomplete light trapping and parasitic losses as major roadblocks in improving the efficiency beyond the current record. Also, we quantify the constraints and requirements for achieving a specified energy conversion efficiency, which is important for a proper design strategy of high efficiency silicon solar cells.

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**#217 - Ge Quantum Dots for Optoelectronic Devices by different synthesis approaches.**

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Semiconductor nanostructures (NS), which exploit the appealing features of a confined system have been widely investigated in the past decades. Beyond the enhanced surface-to-volume ratio or some light management phenomena, one of the most interesting features in nanostructures is the quantum confinement effect (QCE), arising in nanostructures smaller than the exciton Bohr radius (5 nm for Si, 24 nm for Ge). QCE is expected to increase the optical bandgap and the oscillator strength from the bulk values, opening the possibility to tailor the light absorption spectrum, with large potential benefits in photovoltaic applications [1]. Still, up to now this effect has not been largely exploited, since other conditions usually hinder the QCE, as interface related states, large spread in NS size, poor quality of the embedding matrix. In this work, the synthesis and study of Ge quantum dots (2-10 nm in diameter) in SiO<sub>2</sub> matrix grown by plasma-enhanced chemical vapor deposition and magnetron sputtering or low cost liquid phase solution [2](GeBr<sub>2</sub> dissolved in Oleylamine) will be presented, evidencing whether the quantum confinement affects the light-matter interaction and to which level a different synthesis technique affects the physical properties of the QDs. Structural (TEM, RBS, XRD, Raman) and optical (absorption spectroscopy, Tauc analysis) characterizations, and effective mass approximation models are employed to describe the QCE-induced variation of optical bandgap (from 1.0 up to 2.5 eV).

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**#218 - Carrier multiplication in germanium nanocrystals**

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For the first time carrier multiplication (CM) is observed in germanium nanocrystals (Ge NCs): we demonstrate that this effect occurs in self-assembled solid-state dispersion of Ge NCs in a SiO<sub>2</sub> matrix [1]. Ge is of interest since it features a unique band structure with close values of the direct and indirect bandgap energies and a relatively large Bohr radius (~18 nm). Also the technical importance of Ge is growing with its applications for optoelectronics and photovoltaics. CM can significantly enhance the efficiency of energy conversion processes in photo-detectors and solar cells. For solar cells in particular, an overall increased efficiency of up to 44% can be expected for devices that make use of CM [2]. This theoretical maximum is for semiconductors with bandgaps between 0.6 – 1 eV, which is within reach of Ge NCs, with the bulk Ge bandgap of 0.67 eV.

We studied the CM effect in Ge NCs by using ultrafast transient induced absorption spectroscopy. By comparing the photo-induced absorption transients at different pump photon energies, typically below and above the threshold energy for CM, we observed the fingerprint of CM in the form of a fast transient induced by Auger recombination of multiple excitons localized in the same Ge NC. For photoexcitation of 3.5 eV, a CM efficiency of 190% is observed at 2.8 times the optical bandgap of the Ge NCs of 1.25 eV, as determined from their photoluminescence spectrum. For bulk Ge, Koc measured a CM efficiency of 140% for photoexcitation at 3.5 eV, which is at 5.2 times the optical bandgap of bulk germanium [3]. This indicates that the observed CM is considerably more efficient in Ge NCs than in the bulk. We discuss the possibilities for application of Ge NCs in a new generation of highly efficient infrared detectors and future photovoltaics.

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**#219 - Control the growth of hybrid halide perovskites through templating agents towards easy-processable photovoltaic devices.**

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Other Authors: Sofia Masi, Università del Salento Silvia Colella, Università del Salento Andrea Listorti, Italian Institute of Technology (IIT) Giuseppe Gigli, CNR Istituto di Nanotecnologia

Control the growth of hybrid halide perovskites through templating agents towards easy-processable photovoltaic devices. Hybrid halide perovskites have emerged as promising contenders in low-cost devices for next generation optoelectronic devices.[1] Solar cells based on the perovskite-structured light absorber CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> have shown outstanding record photoconversion efficiency of 20.1% [2] that partially originates from the successful development of controlled deposition strategies. Specifically, considerable efforts have been devoted to the development of methods for the preparation of satisfactory perovskite films for a uniform coverage of the photoanode surface.[3] Because of their self-assembly nature, perovskite materials undergo very complex and dynamic equilibria both in solution and in the solid film, thus finding a way to control and affect these equilibria is the key point

toward reproducible processability for large scale production. Among other additives we explored as templating agents for the perovskite growth, we propose the exploitation of polymer matrices as cooperative assembling components for novel perovskite:polymers composites, as powerful tool to predictably tune the film morphology by affecting the self-aggregating properties of the precursors in solution and to make them compatible with roll-to-roll large-area mass production techniques. We demonstrate, through morphological investigations of a series of CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>:Polymer composites, that the polymer's functional groups have a profound effect on the self-assembled nanostructures, while preserving the material structural features. As a proof-of-concept we propose the application of poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV):CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> nanocomposite in polymer solar cell architecture, verify that the employed semiconducting polymer allows the deposition of a very smooth and homogenous layer in one straightforward step. [4] This idea offers a new paradigm for the implementation of polymer/perovskite nanocomposites towards versatile optoelectronic devices combined with the feasibility of mass production. On-purpose designed polymers are expected to suit the nanocomposite properties for the integration in diverse optoelectronic devices via facile processing condition.

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### #220 - Nanohole based Silicon solar cells obtained by molecular doping.

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Quasi-one dimensional (1D) Si nanostructures such as nanowires or nanorods present interesting potentiality for pushing ahead the current limits of Si solar cells thanks to their excellent light harvesting properties or the possibility to form radial junctions which decouple the light direction from the electrical carriers path. 1D structures can be categorized as “positive” structures, namely coming out from substrates to free space, such as the wires, and “negative” structures, which are embedded into the substrate, like for example the nanoholes (NHs). The NHs maintain all the advantages of the positive structures and add an increased robustness to the mechanical stress. This greatly reduces the handling costs and the quantity of waste material thus offering to NHs more space for industrial implementation. In the fabrication processing of nanostructure-based devices the doping step is pivotal. The requirements are: absence of crystal damage, control of doping profile at nm level, possibility to obtain high dopant concentrations and conformality. Doping at the nanoscale with all these requirements has been recently proposed [*Nat. Mat.*, 7(2008) 62]. This method consists in the formation of a self-assembled monolayer (SAM) of dopant precursor molecules via silylation from liquid solutions. The SAM deposited on the Si surface releases the dopant atom from the molecule during the successive thermal treatment and diffuses it into the substrate [PSSA in press]. The technique allows for the formation of n- or p-type doped Si, by properly selecting the precursor source [*MATER SCI ENG B* 178 (2013) 686] also on structured surfaces [*Phys. Stat. Sol. A* 210 (2013) 1564]. The electrical characteristics of the doped layers strictly depend on the physico-chemical properties of the SAM after the silylation [*Phys. Stat. Sol. A* (2015), in press]. An application of the new doping strategy to Si NHs solar cells will be presented. Arrays of SiNHs with  $6 \times 10^{10}$  cm<sup>-2</sup> density, 33nm depth and diameters of 20 nm have been used as top active layers inside the cells [*Sol. En. Mat. Sol. Cells* 132 (2015) 118]. The p-n junctions characteristics have been properly designed in order to have planar or radial junctions with different depths and doping concentrations and it is found that the molecular doping method applied to the Si NHs arrays provides improved photoconversion performance with respect to the reference flat diodes and pave the way to create more efficient nano-electronic devices in the class of new 3D architectures.

### #221 - Study of ZnO nanoparticles synthesized by pulsed laser ablation of a Zn plate in H<sub>2</sub>O

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Zinc oxide (ZnO) nanoparticles (NPs) currently attract much attention stimulated from their use in advanced technologies including photocatalysis, photovoltaics, and bioimaging. These applications take advantage of ZnO optical properties characterized by a direct bandgap  $E_g \approx 3.4$  eV and two emissions at 3.3 eV (exciton related) and at 2.3 eV (defect related). Among the many production methods (chemical reduction of metal ions, sputtering, molecular beam epitaxy, electron beam deposition), pulsed laser ablation in liquid (PLAL) offers a simple and versatile route to synthesize ZnO NPs of extremely high purity. Notably, the solvent not only confines laser-produced species, but also provides a reactive environment to control the metal oxidation.

This work deals with the study of nanomaterials produced by ablation with a ns-pulsed Nd:YAG laser of a Zn plate in H<sub>2</sub>O. The investigation has been carried out by combining complementary techniques to probe the morphology, the structure and the optical properties. Both microscopy (TEM, HRTEM, AFM) images and infrared Raman spectra evidence the formation of ZnO nanocrystals with sizes in the range of tens of nm, the distance between the crystalline planes and the vibrational modes being consistent with

the wurtzite structure. Online absorption (OA) and photoluminescence (PL) measurements carried out during and after PLAL clarify the oxidation dynamics leading to the formation of ZnO. A transient Zn/ZnO core-shell structure is revealed by the coexistence of the OA peak around 5.0 eV due to Zn surface plasmon resonance and optical transitions due ZnO, the OA edge and the exciton-related PL at 3.3 eV. Moreover, we detect the defect-related PL at 2.3 eV rising with a delay (~100 s) from the beginning of PLAL. These kinetics are consistent with a sequence of two steps: an early defect-free superficial oxidation of Zn NPs, followed by a second slower oxidation of the Zn core, leading to sub-stoichiometric ZnO NPs with oxygen vacancies.

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**#222 - Polaritons and the quasiparticle spectral function of graphene on hyperbolic crystals**

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Hexagonal boron nitride (hBN) has received considerable attention in the context of the optical properties of 2D materials. Experimentally, it has been shown that Dirac plasmons in graphene couple strongly to the optical phonons of monolayer hBN [1]. Hybrid plasmon-phonon modes in hBN/graphene/hBN stacks have been investigated by scattering-type near-field optical spectroscopy [2]. Moreover, since hBN is a natural hyperbolic material [3], slabs of hBN support deep subwavelength phonon polaritons [4,5] and display standing Fabry-Pérot phonon-polariton modes [4]. In this work, we theoretically study the coupling of these standing phonon-polariton modes to the plasmons of a two-dimensional massless Dirac fermion liquid in a nearby graphene sheet. We show that a rich spectrum of dispersive plasmon-phonon polaritons emerges, some modes having group velocity as high as the graphene Fermi velocity. These couple strongly with graphene quasiparticles and substantially alter their decay rate and spectral function. Our predictions can be tested in near-field optical and angle-resolved photoemission spectroscopy. References 1. V.W. Brar et al., *Nano Lett.*, 14, 3876 (2014) 2. A. Woessner et al., *Nature Mater.*, (2015) 3. A. Poddubny, I. Iorsh, P. Belov, and Y. Kivshar, *Nature Photon.*, 7, 948, (2013) 4. S. Dai et al., *Science*, 343, 1125, (2014) 5. J.D. Caldwell, *Nature Commun.*, 5, 5221, (2014)

**#223 - Engineering electronic properties in Graphene by substrate effects**

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To create graphene-based devices is of fundamental important to study the electronic properties of graphene when is posed on substrates.

We use first-principles calculations to study the adsorption of graphene on a series of metal and insulating substrates.

The graphene flakes are micrometers in size, sufficiently large to have contacts attached so as to construct field effect transistors.

However graphene has a poor pinchoff as electrons cannot slow down unless a gap is opened.

We studied different interfaces between graphene and hexagonal Boron Nitride to induce the formation of a gap [1] breaking the sublattice symmetry of graphene.

Since electronic transport measurements through a graphene sheet require contacts to metal (Al, Co, Ni, Cu, Pd, Ag, Pt, and Au) electrodes, it is essential to have a full understanding of the physics of metal-graphene interfaces. We used density functional theory calculations to study the doping of graphene and the changes in its electronic structure induced by adsorption on metal surfaces [3,5]. Motivated by the recent progress in preparing and manipulating discrete, essentially atomically perfect graphene layers, we have used electronic structure calculations to explore the spin transport properties of novel grapheme-metal interfaces, predicting perfect spin filtering for ideal metal-graphene-metal/insulator junctions [2,4,6].

As simple example of a commensurate graphene superstructure we considered also graphene on top of hexagonal In<sub>2</sub>Te<sub>2</sub> monolayers [7]. We demonstrated the opening of a Kekule´ band gap of 20 meV, an energy almost as large as kBT at room temperature. Domains of the Kekule´ phase generate the presence of a stable fermionic zero mode with a fractional charge obeying fractional exchange statistics.

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#### #224 - Shielding effect of graphene within ferromagnetic metals

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The magnetic coupling between different magnetic species separated by a graphene layer (G) has recently triggered the interest of the graphene community (1, 2). Concerning the behavior of different ferromagnetic metals (FMs) chemically separated by a G layer, it has been predicted that the coupling can be either ferromagnetic or antiferromagnetic, depending on the choice of the two species (3). This crossover might provide the opportunity for tuning the coupling by varying the chemical composition of the FM/G/FM junction. By recent X-ray magnetic circular dichroism measurements (4) on FM single atoms or islands absorbed on G/Ni at liquid helium temperature, we observed a transition between anti- and ferromagnetic coupling, mainly dependent on the geometrical arrangement of the adatoms at surface. Here we explore the magnetic coupling between FM nano-clusters (Fe, Co, Ni), agglomerating at surface through metal deposition at room temperature, and both G/Co(0001) and G/Ni(111) substrates. The Co and Ni films were grown on W(110) and permanently magnetized *in-situ*. By measuring the dichroic effect of *3p* photoemission lines we detect the remanent magnetization of the substrate, and the sign of the exchange coupling in FM clusters. We show that, in the experimental conditions here examined, the G layer acts as a two-dimensional magnetic screen, quenching the transmission of magnetic interaction towards the FM clusters.

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#### #225 - CdS/graphene hybrid photodetectors

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The application of graphene to photodetectors in the visible and near UV range suffers from low absorption of this gapless 2D material [1]. Among the different approaches to improve the performance in terms of responsivity, hybrid devices based on graphene and sensitizer materials have proved to be a promising solution to this problem. In particular the use of colloidal semiconductor nanocrystals [2] has given very good results [3,4]. In the hybrid system, the light generates charges in the semiconductors, which are transferred to the graphene layer inducing a sizeable change in the current flowing through it. In this way, it is possible to exploit the high absorption of the nanocrystals and the high mobility in graphene. However, the relaxation processes of the photogenerated charges can be slow and limit high frequency performance of the device. It is also possible to tune the response via the charge density in graphene, using a back-gated sample; in the same manner, the sign of the photocurrent can be switched from positive to negative, because of the ambipolar character of graphene [5].

In this contribution, we will report on photodetectors fabricated with CVD graphene transferred onto a n-Si/SiO<sub>2</sub> substrate, to be used as a back gate; a thin film of CdS nanocrystals is deposited onto the sample by spin coating. The spectral response of the device follows the absorption of the nanocrystals, giving high sensitivity in near UV range. The devices show a maximum responsivity of about  $4 \cdot 10^4$  A/W. Using a pulsed laser at 349 nm, we could detect ns-pulses up to 2 kHz repetition rate, thus demonstrating that fast relaxation processes can be exploited.

To better understand the physical processes in the hybrid system, we will discuss the effective mechanisms of charge transfer from nanocrystals to graphene, and the role of surface states and adsorbed molecules [6-8]. Finally, we will introduce models for the photodetection, based on the experimental response of the device as a function of light power and pulse repetition rate.

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#### #226 - Optical response of epitaxial silicene on silver probed by transition reflectance spectroscopy

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The recent integration of silicene in field-effect transistors (FET) opened new challenges in the comprehension of the chemical and physical properties of this elusive two-dimensional allotropic form of silicon. Intense efforts have been devoted to the study of the epitaxial Silicene/Ag(111) system in order to elucidate the presence of massless Dirac fermion in analogy with graphene; strong hybridization effects in silicene superstructures on silver have been invoked as responsible for the disruption of  $\pi$  and  $\pi^*$  bands. In this framework, the measured ambipolar effect in silicene-based FET characterized by a relatively high mobility, points out to a complex physics at the silicene-silver interface, demanding for a deeper comprehension of its details on the atomic scale.

The present work aims to elucidate the role of the Ag(111) metallic support in determining the physical properties of the Si/Ag two-dimensional interface, by means of optical techniques combined with theoretical calculations of the optical response of the supported system. The silicene/Ag(111) spectra, which turn out to be strongly non-additive, are analyzed in the framework of theoretical density functional based calculations allowing us to single out different contributions. Electronic transitions involving silver states are found to provide a huge contribution to the optical absorption of silicene on silver, compatible with a strong Si-Ag hybridization. The results point to a dimensionality-driven peculiar dielectric response of the two-dimensional-silicon/silver interface, which is confirmed by means of Transient-Reflectance spectroscopy. The latter shows a metallic-like carrier dynamics, (both for silicene and amorphous silicon), hence providing an optical demonstration of the strong hybridization arising in silicene/Ag(111) systems.

#### #227 - Pseudo-Yagi-Uda antenna made of graphene for terahertz light

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Reflection, transmission, and absorption spectra of stacked graphene microribbons in the terahertz region were simulated by the finite element method. The microribbons, which resonantly couple with terahertz light through the excitation of plasmons, were stacked with micrometer-scale vertical spacing ( $\sim 0.1 \times$  wavelength or larger). Reflection and absorption spectra were found to strongly depend on the direction of incident light (forward or backward incidence) when the resonance frequencies in each layer were made slightly different by changing the ribbon width or the chemical potentials. At a certain frequency, light reflection is almost completely suppressed only for one incidence direction. Our simulation showed that when reflection was almost completely suppressed, plasmons were almost equally excited in the upper and lower ribbons and the two reflected waves interfered in the opposite phase. From these results, the high directivity is considered to be due to the phasing effects of electromagnetic waves like in a Yagi-Uda antenna. This plasmonic graphene antenna can be much smaller than a conventional Yagi-Uda antenna owing to the fact that the wavelength shrinks when the terahertz light excites a plasmon in a graphene pattern. The backward/forward ratio of the reflectance reaches 290 for two-layer stack and 1260 for three-layer stack. By combining the large optical anisotropy and the field-effect-induced tunability of graphene, it would be possible to fabricate reconfigurable optical devices whose optical properties and their anisotropy are widely controllable.

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#### #228 - Ambient stability of oxygen p-doped graphene

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Graphene (Gr), a single layer of graphite, has attracted in recent years many interests of researchers for its potential electronic and optoelectronic applications. For these aims a wide research has been devoted to prepare large-area un-defective materials, growing them on metal substrates (such as Cu, Ni) using Chemical Vapor Deposition (CVD), and to successively transfer them onto specific substrates, like SiO<sub>2</sub>/Si, for device construction. In addition, for the electronic tasks, detailed studies have been dedicated to the doping of graphene to specifically tune its carrier density. It has been so shown that doping could be induced, apart that during the synthesis, also by post growth procedures, among which, thermal treatments in controlled atmosphere. In this context, the investigation of doping efficiency and stability is of particular concern for the final material conductivity features aiming also to separate those aspects strictly related to the physical properties of graphene, like defects content and morphology, from those related to the graphene substrate interaction.

Aim of the present work is to characterize by micro-Raman spectroscopy and Atomic Force Microscopy the features of the p-Type doping efficiency of Gr grown on SiO<sub>2</sub>/Si substrates by thermal treatments in controlled atmosphere of oxygen up to 10 bar or in vacuum, and to evaluate the post processing stability. A comparison of storage in air or in vacuum is also considered to highlight those not stable effects. By temperature scans it is found an onset temperature for doping of about 140°C and doping stability in vacuum up to 300°C. A partial recovery towards undoped Gr is found by storage in air as contrasted to storage in vacuum. This aspect suggests that stable traps for oxygen dopant are present on Gr or in the Gr/substrate interlayer but their reactivity with ambient molecules (N<sub>2</sub>, H<sub>2</sub>O, CO<sub>2</sub>,.....) originates the changes evidencing also exploitable potentialities for sensing applications.

### #229 - Atomistic simulation of graphene processes

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Here we present a generic multi-scale atomistic simulation method of different graphene manipulation processes based on a Kinetic Monte Carlo approach formulated on augmented lattices. The stochastic simulation method is calibrated by "ab-initio" calculations of stable and meta-stable configurations and eventually coupled to the continuum simulation of the kinetics and the reactions in the gas phase when it is relevant for some particular cases. We consider the following cases: thermal annealing of defects and impurities in graphene, Chemical Vapour Deposition (CVD) and selective Si evaporation synthesis techniques are considered on metal (Cu) and silicon carbide (SiC) substrates. It is noteworthy that in the latter case the inner structural transition from the SiC crystal structure to the graphene lattice structure is also simulated. Defects and impurity evolution show peculiar characteristic due the effects of effective coalescence barriers. Kinetics of the deposited atomic layer kinetics proceeds by islands' nucleation and (Ostwald ripening type) growth in the case CVD processes; whilst structural transition from SiC to graphene is mediated by disordered weakly bounded carbon-carbon configurations in the carbon rich regions generated by the selective Si sublimation. Simulations of the nitrogen atoms (Ns) incorporation during the CVD growth predict a sub-lattice symmetry breaking due the preferential sitting of N atoms in perfect zig-zag configuration at the growing edges. Quantitative predictions of the process evolution in term of crystal state and defects' generation as a function of the initial state and the process's parameters (temperature, pressure, gas flows) can be obtained and readily compared with experimental structural characterization of processed samples.

**#230 - Chiral optofluidics**

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Chirality in soft matter is emerging as a tool to address innovative concepts in materials science, colloidal systems, optical and photonics devices, optomechanics, optofluidics etc..

Two examples are presented; the first one refers to chiral optofluidic devices and the second one to optofluidics strategies for nanoparticles assembling and manipulation.

We investigate the optical forces and torques on spherical polymeric particles with chiral arrangement of the inner structure consisting of supramolecular helices (left or right-handed). The methodological approach used for micro-particles preparation is such that the helical arrangement self-organizes in precursor cholesteric liquid crystal droplets by proper selection of a chiral dopant. The helical pitch is adjusted from nanometer to micrometer range by means of the dopant concentration. The helicoidal arrangement can lead to a shell structure of the refractive index and to a selective Bragg phenomenon that makes them to behave as chiral spherical mirrors for light propagating along the helical axis and wavelength within the stop band. The circularly polarized light component having the same handedness of the chiral arrangement is reflected leaving its spin state unchanged. On the contrary, the light having opposite handedness is transmitted unaffected. The sign and strength of the optical force depend on the particles reflectance. Moreover, in contrast to conventional reflecting particles, these chiral particles can be set in rotation because of the transfer of spin angular momentum. We investigate the tunability and the coupling of the optical forces and torques by controlling the amount of the reflected light. Chirality-controlled optical trapping and manipulation opens novel strategies for optomechanics and optical sorting.

We exploit chiral photosensitive materials to move nanoparticles-charged disclination lines in anisotropic chiral fluids. We demonstrate the ability to trap nanoparticles and to manipulate them at large scale by low power incoherent light. The chirality is introduced at two levels, by the boundary architectures and by a photosensitive chiral dopant. The first permits to design the topological defects templates, the second to move nanoparticles-charged disclination lines without disrupting them. Full reconfigurability and time stability make this strategy attractive for future developments and practical applications.

We acknowledge the MPNS COST Action 1205 "Advances in Optofluidics: Integration of Optical Control and Photonics with Microfluidics" for supporting these activities.

**#231 - Red Blood Cell behaves as an adaptive liquid micro-lens**

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Red Blood Cells (RBCs) behave as micro-lenses with specific focal lengths, magnification and tunability properties.

Erythrocytes, in their mature state and under physiological and healthy conditions, are flexible biconcave disks with homogeneous distribution of the refractive index. By an optical point of view, the lack of nucleus and organelles allows to model RBC as a sort of disk-shaped micro-structure envelope exploitable as micro-lens. The focal length, the aberrations and the magnification are theoretically predicted and experimentally demonstrated.

Furthermore, RBCs membrane present a great deformability in comparison to other cells so that the focal length can be tuned by changing the RBC shape. A complete analogy between RBC and adaptive lens exists. RBC morphology variation is achievable by triggering the liquid buffer osmolarity thus permitting swelling from biconcave microfluidic disk (Volume = 90fL) up to a sphere (Volume = 150fL). Taking into account the average refractive indexes of RBCs and buffer, the focal length changes from negative value (about -6.0 $\mu$ m) to positive ones (about 10 $\mu$ m) when the transition between discocyte and spherocyte is induced.

A direct application of this discovery is in terms of diagnosis. Indeed, many blood disorders are reflected in RBC shape anomalies (for examples Sickle-cell disease, Malaria, Spherocytosis and Anemias). Such modifications in the cell shape is detectable by the optical properties of the RBC. Indeed, healthy erythrocytes present unique optical characteristics and any differences can be evaluated by the analysis of the wavefront aberrations as in adaptive optics technology.

**#232 - Integrated opto-microfluidics platforms in lithium niobate crystals for sensing applications**

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Microfluidic technology holds great promise as it can perform typical laboratory applications using a fraction of the volume of reagents in significantly less time. Applications for microfluidics have significantly advanced from its root in micro-analytical chemistry to include high throughput screening, biological analysis of cells and proteins and reaction kinetics and mechanism

studies [1]. Although novel microfabrication techniques are continuously being developed, the development of micro-devices with appropriate fluidic interfacing scheme is still under debate to get lab-on-chip system [2-3]. Among the others, even lithium niobate (LiNbO<sub>3</sub>) crystals have been proposed in microfluidics since allows for high efficient acoustic waves generation to move droplets on the substrate in a very controlled way, flow mixing and pumping, pyro-electric and photo-galvanic particle and droplet actuation. Quite surprisingly, all the above mentioned applications were realized without producing a microfluidic circuit directly on LiNbO<sub>3</sub> substrates and without the integration of optical sensing stages, although it is a material thoroughly exploited in the photonic and integrated optics industry. Recently lithium niobate has been also proposed as candidate for application in opto-microfluidic technology [4-6], thus combining the tools typical of microfluidics with the potentialities offered by this material. In this work, the recent results on the integration of a microfluidic circuit with optical waveguides will be presented with particular care to the exploitation of an integrated input waveguide to illuminate the fluid in micro-fluidic channel and how to collect the transmitted light by way of output waveguide engraved on the same substrate. By monitoring the optical transmission spectrum, the analysis of the optical response of the fluid components can be achieved, with applications to optical sensing platforms in a lab-on-chip system entirely based on LiNbO<sub>3</sub> substrate.

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### #233 - Studying and controlling drop motion on inclined surfaces

*Silvia Varagnolo - CNISM and University of Padova, Dept. Physics and Astronomy "G. Galilei"*

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We present an overview about the motion of drops on inclined surfaces, including different liquids (newtonian and non-newtonian fluids) and substrates having homogeneous and chemically heterogeneous surfaces.

The sliding of water drops down homogeneous surfaces is compared to that of polymeric solutions featuring different non-newtonian behavior (shear thinning or normal stress difference effects) [1]. A significant deviation between newtonian and non-newtonian sliding drops appears at high inclination angles and is stronger at higher polymer concentration: for newtonian drops the steady sliding velocity scales linearly with the down plane component of the gravity force, while non-newtonian drops follow this linear dependence at small inclination angles and at high inclinations a sublinear trend or a plateau appear.

Similar measurements have been also performed with water drops on chemically heterogeneous surfaces formed by hydrophilic and hydrophobic domains of different shape (stripes, squares and triangles) arranged in different patterns [2-4]. The wettability contrast between the hydrophilic and hydrophobic regions causes the drop to undergo a particular stick-slip dynamics characterized by steps of the front and rear contact points and a mean velocity depending on the pattern geometry. These studies show that chemical patterns can be successfully exploited to passively control drop velocity.

An active method to control drop motion on inclined homogeneous surfaces involves the application of vertical acoustic vibration to the substrate [5]. According to the combination of amplitude and frequency of vibration, a drop can slide down, be pinned or even climb up against gravity. The liquids investigated are water and newtonian aqueous solutions of glycerol, isopropanol and ethanol. For all these fluids the behavior is similar except for the more wetting solutions that cannot climb.

All these experimental results have been completed and confirmed by numerical simulations.

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### #234 - Role of viscoelasticity in droplet formation inside a microfluidic T-junction

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The progressive break-up of a fluid thread into a number of small drops [1] is a rich physical phenomenon which impacts many applications [2,3]. In particular, droplet-based microfluidic devices have gained a considerable deal of attention, due to their importance in studies that require high throughput control over droplet size. Common droplet generator designs used in these

devices are T-shaped geometries [4,5] and flow-focusing devices [6–8]. With a few exceptions [10–12], previous research has been mainly restricted to Newtonian fluids. However, the processing of biological fluids with high molecular weight macromolecules inevitably results in considering a non-Newtonian viscoelastic behaviour. Consistently, the use of viscoelastic liquids in flow-focusing devices [10,11] or T-junction geometries [12] has recently taken into account, but needs further investigation. Here we investigate the role of viscoelasticity in droplet formation in a microfluidic T-junction, where newtonian oil droplets are dispersed in a non-newtonian aqueous polymer solution of Polyacrylamide (PAA), which displays normal stress effects, at different concentrations in the semidilute regime. The experiments are performed in a hydrophilic chip made in NOA, which enables to have oil-in-water droplets if a surfactant is added to the continuous phase [9]. Numerical simulations with lattice Boltzmann and FENE-P model [13] are performed on the same system, enabling us to visualize the normal stress distribution in the viscoelastic continuous phase. The simulations display a normal stress build-up upstream of the emerging droplet. This contributes as an extra force in the droplet break-up resulting in smaller droplet sizes, in qualitative agreement with the experimental observations. References [1] J. Eggers, *Rev. Mod. Phys.* 69 (1997) 865. [2] G.F. Christopher, S.L. Anna, *J Phys D Appl Phys* 40 (2007) R319. [3] S. Teh, R. Lin, L. Hung, A. Lee, *Lab. Chip* 8 (2008) 198. [4] M.D. Menach, P. Garstecki, F. Jousse, H.A. Stone, *Jour. Fluid. Mech.* 595 (2008) 141. [5] M.D. Menach, *Phys. Rev. E* 73 (2006) 031505. [6] H. Liu, Y. Zhang, *J. Appl. Phys.* 106 (2009) 034906. [7] H. Liu, Y. Zhang, *Physics of Fluids* 23 (2011) 082101. [8] L. Derzsi, M. Kasprzyk, J.P. Plog, P. Garstecki, *Phys. Fluids* 25 (2013) 092001. [9] E. Piccin, D. Ferraro, P. Sartori, E. Chiarello, M. Pierno, G. Mistura, *Sensors and Actuators B.* 196 (2014) 525–531. [10] P.E. Arratia, J.P. Gollub, D.J. Durian, *Phys. Rev. E* 77 (2008) 036309. [11] B. Steinhaus, A.Q. Shen, R. Sureshkumar, *Phys. Fluids* 19 (2007) 073103. [12] J. Husny, J. Cooper-White, *J. Non-Newton. Fluid Mech.* 137 (2006) 121. [13] A. Gupta, M. Sbragaglia, A. Scagliarini, *Journal of Computational Physics* 291 (2015) 177–197.

### #235 - Catalytic oxygen production mediated by smart capsules to modulate elastic turbulence under a laminar flow regime

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Movement of fluids and an efficient mixing are the first step to perform a number of chemical and biological microfluidic processes. The progress in microfluidic technologies has made possible the complicated manipulation of solutions at the microscale [1,2], but many devices have relied on external instruments such as microsyringe pumps or power sources. Moreover, liquid flow in microchannels is completely laminar and uniaxial, with a very low Reynolds number regime [3,4]. To increase fluid mixing, complex three-dimensional networks inducing chaotic advection have to be designed. Alternatively, turbulence in the liquid can be generated by active mixing methods (magnetic, acoustic waves, etc.) or adding small quantities of elastic materials (viscoelastic polymers) to the working liquid [5,6].

We have used polyelectrolytemultilayer capsules (PMCs) embodying a catalytic polyoxometalate complex ( $Ru_4POM$ )[7] to propel fluids inside microchannels and to create elastic turbulence. The overall effect is enhanced and controlled by feeding the polyoxometalate-modified capsules with hydrogen peroxide,  $H_2O_2$ , thus triggering an on-demand propulsion due to oxygen evolution resulting from  $H_2O_2$  decomposition [7]. The capillary dynamics of the aqueous mixtures with different concentrations of  $H_2O_2$  in a microchannel have been analyzed and this study has allowed the quantification of some structural parameters of motion such as speed, pressure, viscosity, and Reynolds and Weissenberg numbers. The increases in fluid speed as well as the capsule-induced turbulence effects are proportional to the  $H_2O_2$  added and therefore dependent on the kinetics of  $H_2O_2$  dismutation [8].

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# September 30

**Molecular Biophysics I** **Antonio Cupane**

**Statistical Mechanics of Active Matter** **Duccio Fanelli**

**Light Manipulation** **Livio Gianfrani**

**Plasma Physics IV** **Alessandro Cardinali**

**Magnetism and Spin related Phenomena III** **Ilaria Bergenti**

**Thin films, Devices, Weak Superconductivity and Applications** **Carlo Ferdeghini**

**Topological Insulators** **Silvia Picozzi**

**Non Linear Optics** **Paolo De Natale**

**Photonic and plasmonic materials and devices** **Francesco Priolo**



**#236 - Small-angle X-ray scattering from biomacromolecular solutions**

*Dmitri Svergun (I) - EMBL Hamburg*

Small-angle X-ray scattering (SAXS) experiences a renaissance in the studies of macromolecular solutions allowing one to study the structure of native particles and complexes and to rapidly analyze structural changes in response to variations in external conditions. Novel data analysis methods significantly enhanced resolution and reliability of structural models provided by the technique [1]. Emerging automation of the experiment, data processing and interpretation make solution SAXS on high brilliance synchrotron sources a streamline tool for large scale structural studies in molecular biology. The method provides low resolution macromolecular shapes *ab initio* and is readily combined with other structural and biochemical techniques in hybrid approaches. Of special interest is the joint use of SAXS with the high resolution methods like crystallography and NMR, but also with complementary biophysical and biochemical techniques. Rapid validation of predicted or experimentally obtained high resolution models in solution, identification of biologically active oligomers and addition of missing fragments to high resolution crystallographic models are possible. For macromolecular complexes, quaternary structure can be effectively analyzed in terms rigid body movements/rotations of individual subunits, if their structures are available. SAXS can also be applied to characterize the solution states of flexible and intrinsically disordered macromolecules. The methods will be illustrated by examples of recent applications and the perspectives of the synergistic use of SAXS with other techniques in structural biology will be reviewed.

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**#237 - Phototransformable fluorescent proteins: a mechanistic view.**

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Phototransformable fluorescent proteins (PTFPs) have received considerable attention in recent years because they enable many new exciting modalities in fluorescence microscopy and biotechnology. Upon illumination with proper actinic light, PTFPs undergo long-lived transitions between various fluorescent or nonfluorescent states, resulting in processes known as photoactivation, photoconversion or photoswitching. These processes come in addition to stochastic photoblinking and irreversible photobleaching, which universally characterize fluorescent molecules. The highly complex photophysical behavior of PTFPs can be investigated at the molecular scale by a combination of X-ray crystallography, in crystallo optical spectroscopy (UV-vis absorbance, fluorescence and Raman), mass spectrometry and simulation methods such as quantum-chemistry/molecular-mechanics hybrid approaches. In this way, it is possible to decipher the subtle conformational dynamics driving phototransformations in PTFPs, eventually facilitating the rational engineering of better performing markers for advanced nanoscopy or biotechnological applications. Based on our studies of IrisFP, a fascinating PTFP which exhibits combined green-to-red irreversible photoconversion and on-off reversible photoswitching in both its green and red states, we will detail how photoactivated structural dynamics in PTFPs control their complex photophysics. We will in particular focus on mechanisms that lead to photoblinking and photobleaching.

**#238 - The Effect of Room-Temperature Ionic Liquids on the Structure and Dynamics of Bio-Membranes and their Hydration Water: a Neutron Scattering and Computer Simulation Study**

*Antonio Benedetto - Paul Scherrer Institut (PSI)*

*Other Authors: Pietro Ballone (Center for Life Nano Science and Phys. Dep., Roma La Sapienza, Italy)*

The molecularly thin layer of water in direct contact with bio-molecules in a physiological environment plays a major role in determining their properties and functions. In this context, water is a shorthand notation for “*water electrolyte solution*”, since almost without exception a variety of ions dissolved in water are needed to ensure the stability of bio-systems, greatly contributing to their complex behaviours.

In recent years, the development of compounds of the so-called room-temperature ionic liquid (RTIL) family has enormously expanded the number of ionic systems that could be used to modify the properties of the interfacial water, and thus to affect the behaviour of bio-systems.

Our study concerns the microscopic mechanisms underlying RTIL effects on biosystems (e.g. phospholipid bilayers, proteins, and nucleic acids) through their hydration water, and relies on the combination of neutron scattering and molecular dynamics (MD) simulations.

We present the results for the interaction of imidazolium-based RTILs with phospholipid bilayers [1,2]. Neutron reflectometry and MD simulations confirm the tendency of cations to be absorbed into the lipid phase, enhancing the penetration of water into the bilayer. Neutron scattering and MD reveal apparent changes in the relaxation time of water in close contact of the lipid head upon addition of RTILs, that reflect phase changes in the structure and dynamics of the system.

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### #239 - New insight into the function of bacterial amyloids

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Accumulating evidence indicates that RNA metabolism components assemble into supramolecular cellular structures to mediate functional compartmentalization within the cytoplasmic membrane of the bacterial cell. This cellular compartmentalization could play important roles in the processes of RNA degradation and maturation. These components include Hfq, the RNA chaperone protein, which is involved in the post-transcriptional control of protein synthesis mainly by the virtue of its interactions with several small regulatory noncoding RNAs. The *E. coli* Hfq is structurally organized into two domains. An N-terminal domain that folds as strongly bent  $\beta$ -sheets within individual protomers to assemble into a typical toroidal hexameric ring. A C-terminal flexible domain, that encompasses about one-third of the protein, seems intrinsically unstructured. RNA binding function of Hfq mainly lies within its N-terminal core, whereas the function of the flexible domain remains controversial and largely unknown. In this paper, thanks to the structural studies with biochemical and biophysical methods, we demonstrate that the Hfq C-terminal region has an intrinsic property to self-assemble into long amyloid-like fibrillar structures *in vitro*. We show that normal localization of Hfq within membrane-associated coiled structures *in vivo* requires this C-terminal domain. This finding establishes for the first time a function for the hithertopuzzling C-terminal region, with a plausible central role in RNA transactions.

### #240 - Protein and hydration water dynamics in folded and intrinsically disordered proteins

Giorgio Schirò - CNRS Institut de Biologie Structurale

Hydration water is the natural matrix of biological macromolecules and is essential for their activity in cells. The coupling between water and protein dynamics has been intensively studied, yet it remains controversial. We combined protein perdeuteration, neutron scattering and molecular dynamics simulations to explore the nature of hydration water across the so-called protein dynamical transition [1], in the intrinsically disordered human protein tau and the globular maltose binding protein. We generalized the notion that the translational diffusion of water molecules on a protein surface promotes the large-amplitude motions of proteins that are required for their biological activity [2]. We also studied the dynamics of hydration water at the surface of fibers formed by the full-length human tau, one of the pathological hallmarks of Alzheimer disease. We found that water is more mobile in tau fibers than in nonaggregated tau, thus corroborating that methodologies sensitive to the diffusion of water, such as diffusion magnetic resonance imaging, could be used to diagnose Alzheimer patients in an early stage of the disease [3].

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### #241 - MediaChrom: a new class of versatile polarity-sensitive dyes for imaging applications

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Modern biological research needs a continuous development of new fluorescent dyes, to be used as markers or probes, characterized by improved performances. These molecules should allow a highly specific and sensitive monitoring for a wide range of biological processes. A particular class of dyes, called environment-sensitive dyes, are able to change their spectroscopical properties in response to the change of physico-chemical features of their environment. Among them, polarity-sensitive dyes (also called solvatochromic dyes) have the unique feature to display a different emission maximum as a function of the environment polarity. This property makes them the ideal probes to monitor the local properties of particular cell districts, as well as different types of biomolecular interactions (e.g., peptide-nucleic acid, protein-protein, and peptide-lipid interactions).

Several polarity-sensitive dyes have been developed, but most of them are far to meet simultaneously all the optimal spectroscopic requirements for biological applications, i.e., a strong solvatochromism, absorption in the visible range, high extinction coefficient, high quantum yield, good photostability.

We designed a new class of polarity-sensitive dyes, named MediaChrom, that absorb and emit light in the visible range with good extinction coefficient and quantum yield. MediaChrom proved to be highly sensitive to the environment polarity and easily conjugated to proteins and peptides for directing them to defined biological targets.

**#242 - Protein-Lipid Interface in Na,K-ATPase Membranes by pulsed EPR**

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The Na,K-ATPase active transport enzyme is an integral protein of the plasma membrane that is responsible for maintaining ionic balance in eukaryotes.

Spin-echo EPR is used to study the profiles of the librational motion and water penetration in Na,K-ATPase membranes by using lipids labelled at selected C-n positions along the acyl chain. The torsional librations in the protein are coupled to librational fluctuations of the lipid chains and, at the same time, the protein influences the characteristics of the hydrophobic barrier in the membrane.

Lipid librations at the protein interface have a flat profile, whereas librational fluctuations of the bilayer lipids increase progressively from C-9 onwards, then levelling off towards the terminal methyl end of the chains. This difference is accounted for by an increased torsional amplitude at the chain ends in bilayers, whilst the amplitude remains restricted throughout the chain at the protein interface with a limited lengthening in correlation time. The temperature dependence of chain librations at the protein interface strongly resembles that of the spin-labelled protein side chains. This suggests that solvent-mediated transitions in the protein are coupled by fluctuations in the lipid environment.

In native Na,K-ATPase membranes and bilayers of the extracted membrane lipids, the D<sub>2</sub>O-ESEEM intensities decrease progressively with position down the fatty acid chain. The profile decreases sharply in the lipid bilayers and is much broader in membranes. For positions at either end of the chains, the D<sub>2</sub>O concentrations at the interface are greater than in the lipid bilayer. In particular, there is a significant water concentration at the membrane mid-plane adjacent to the protein. The polarity and concentrations of intramembrane water at the lipid interface with integral proteins are higher and the hydrophobic barrier is less sharp than in the lipid-bilayer regions of biological membranes.

**#243 - Structural and functional alterations of connexin 32 channels with a C-terminal truncation causing Charcot-Marie-Tooth disease.**

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The X-linked form of Charcot–Marie–Tooth disease (CMT1X) is the second most common form of hereditary motor and sensory neuropathy, for which there is no cure. Over 400 different mutations associated with CMT1X have been identified in the gene encoding connexin 32 (Cx32), a tetraspan membrane protein which forms hemichannels and reflexive junctional channels in the Schwann cell myelin sheath, providing critical, fast radial pathways for the passage of ions and signaling molecules. A key feature that has emerged from the huge number of studies on normal (wild-type, WT) and mutated Cx32 expression and function has been the identification of so-called functional mutations, which retain the basic capacity to ensure electrical coupling but display still unknown abnormalities causing CMT1X.

In this study we performed experiments in Cx32-transfected HeLa cells to determine whether a functional channel with C-terminal truncation (R220stop) could indeed present with abnormal expression, permeability or gating properties. Interestingly, mutant hemichannels exhibited altered conductance sub-states and abnormal openings during cell depolarization or cytosolic Ca<sup>2+</sup> increase. Our Cx32 hemichannel model, the first based on molecular dynamics simulations and derived by homology modelling from the recent Cx26 crystallographic structure of Maeda et al. (Nature, 2009), suggests that lack of the C-terminal can alter the gating properties of the channel by increasing the mobility of the entire cytoplasmic region. Immunofluorescence analysis combined with electrophysiology experiments highlighted also defective formation of Cx32-R220stop junctional plaques (gap junctions, GJ), by a 2.5 fold reduction of the GJ area in respect to WT, due to presumed impaired trafficking of the mutant protein. By contrast, FRET experiments combined with dual patch-clamp revealed that the single GJ channel permeability to ions (K<sup>+</sup>), second messengers (cAMP) and larger exogenous solutes (lucifer yellow) is similar in the WT and R220stop.

Altogether, these results clarify the physiological function of Cx32 C-terminal domain and provide a mechanistic explanation for CMT1X pathogenesis, as defective hemichannel opening or plaque formation may damage the cell through perturbation of ionic gradients and metabolite exchange between the Schwann cell and its axon.

**#244 - Dense active nematics***Julia Yeomans (I) - University of Oxford*

Active systems, such as bacterial suspensions and the cytoskeleton, driven by molecular motors, provide their own energy and hence operate out of thermodynamic equilibrium. Continuum models describing active systems are closely related to those describing liquid crystal hydrodynamics, together with an additional 'active' stress term. I shall discuss recent results from simulations of dense active nematics and discuss their applicability to cell motility and cell division.

**#245 - Hydrodynamic trapping of swimming bacteria by convex walls***Roberto Di Leonardo (I) - CNR-NANOTEC & Dip. Fisica Sapienza*

Swimming bacteria display a remarkable tendency to move along flat surfaces for prolonged times. This behavior may have a biological importance, but can also be exploited using microfabricated structures to manipulate bacteria. The main physical mechanism behind the surface entrapment of swimming bacteria is however still an open question. By studying the swimming motion of *Escherichia coli* cells near microfabricated pillars of variable size, we show that cell entrapment is also present for convex walls of sufficiently low curvature. Entrapment is however markedly reduced below a characteristic radius. Using a simple hydrodynamic model, we predict that trapped cells swim at a finite angle with the wall and that a precise relation exists between the swimming angle at a flat wall and the critical radius of curvature for entrapment. Both predictions are quantitatively verified by experimental data. Our results demonstrate that the main mechanism for wall entrapment is hydrodynamic in nature, and show the possibility of inhibiting cell adhesion, and thus biofilm formation, using convex features of appropriate curvature.

**#246 - Phase separation and coarsening in an active dumbbell system***Giuseppe Gonnella (I) - Università di Bari*

Active matter refers to systems driven out of equilibrium by internal or external energy sources continuously transformed into movement or work on the environment. Active matter systems are characterized by many peculiar properties not present in their passive counterparts, like clustering, anomalous diffusion, giant fluctuations, unexpected rheological properties.

Here, we will shortly review the results obtained from the study of a two-dimensional system of active dumbbells, introduced as a paradigmatic example of a system of non symmetrical brownian particles with self-propulsion.

Each dumbbell is composed by two colloids kept together

by a rigid spring, with an excluded volume interaction modeled through a Weeks-Chandler-Anderson (WCA) potential.

They are immersed in an implicit solvent modeled by the

Langevin equation. The activity or self-propulsion is modeled by a constant force acting on the principal direction of the dumbbell. This model wants to be a coarse-grained characterization of the behavior of simple bacteria

and tries to study them from a statistical point of view. Hydrodynamic interactions are ignored.

As in a fluid of spherical swimmers, we find that activity triggers a nonequilibrium phase separation if the

density exceeds a critical threshold and if the Peclet number is high enough. We study the kinetics of the aggregates of dumbbells in the phase separated region. The clusters spontaneously break chiral symmetry and rotate; they also display a nematic ordering with spiral patterns. We can also determine the growth law for the size of these clusters.

**#247 - Polymer dynamics in viscoelastic, active baths***Carlo Vanderzande - Hasselt University**Other Authors: Hans Vandebroek, Hasselt University*

We study the dynamics of an ideal polymer chain in viscoelastic materials and in the presence of active forces. We determine the motion of the centre of mass and of individual monomers. We find that on time scales that are comparable to the persistence time of the active forces, monomers can move superdiffusively while on larger time scales subdiffusive behaviour occurs. We quantify the difference between this subdiffusion and that in absence of active forces. We show that the polymer swells in response to active processes and determine how this swelling depends on the viscoelastic properties of the environment. We compare our results to recent experiments on the motion of chromosomal loci in bacteria.

**#248 - Boundary information inflow enhances correlation in flocking systems***Francesco Ginelli - University of Aberdeen*

It is an obvious statement that many biological systems do not operate in isolation, but constantly interact with a complex external environment. In this talk we address the specific example of a flock interacting with a dynamic external environment. Environmental perturbations directly affect the flock boundary, and are then transferred to the bulk via local interactions (social forces).

By means of numerical simulations and theoretical calculations, we show that this information inflow triggers long-range spin-wave modes, thus giving rise to *anomalously* long-ranged correlations in velocity fluctuations.

This results is compared with experimental data in 3D starlings flocks, showing that the velocity fluctuations correlation function is not only scale-free -- as expected in any system spontaneously breaking a continuous symmetry -- but also very slow decaying. In fact, the exponent ruling the decay of the velocity correlation function,  $C(r) \sim r^g$ , is found to be vanishing in both the boundary-perturbed model and the experimental data.

#### #249 - Spatial Confinement of Bacterial Solutions

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A systematic investigation of the spatial distribution of two different types of bacteria, *E. Coli* and *P. Aeruginosa*, confined between two flat walls having a separation of tens of microns was carried out by counting motile bacteria at different distances from the bottom wall [1]. A custom tracking software was developed in order to distinguish swimming bacteria from passive ones. In agreement with previous studies [2], an enhancement of the density of motile bacteria close to the walls was observed. Different concentrations of bacteria in suspension and different wall separations, ranging from 100  $\mu\text{m}$  to 250  $\mu\text{m}$ , were tested. The same systems were also studied by means of numerical simulations, using a collection of self-propelled rod-like particles interacting only through steric interactions. Numerical results are in agreement with the experimental profiles suggesting that steric interactions are sufficient to produce the density enhancement effect.

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#### #250 - Freezing of Hard Colloidal Cubes

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Nucleation of Hard Colloidal Cubes

Carina Karner and Christoph Dellago

Abstract

Currently, research on hard anisotropic colloids is receiving a lot of attention from various experimental and theoretical groups in the soft matter community, partly due to the availability of new fabrication techniques making it possible to produce colloidal particles with various anisotropic shapes or interactions [1]. Recent results obtained from computer simulations and theory indicate that many three dimensional hard anisotropic particles of polyhedral shape exhibit a first order phase transition from an unordered fluid to an ordered crystal. Hard colloidal cubes belong to this class of particles and have recently been studied numerically [2] as well as experimentally [3].

Unlike isotropic particles, cubic particles have to assume not only positional but also orientational order as they crystallize. Therefore the natural question to ask is how the interplay of orientational and translational degrees of freedom influences the course of the transition.

In order to gain insight into the dynamics of the freezing transition, we employed kinetic Monte Carlo in combination with rare event sampling methods. Using free energy and nucleation rate calculations, we show that even at low over-pressuring, cubic colloids transition extremely fast from the metastable liquid to the cubic crystal. Our findings provide further evidence that hard colloidal cubes assume first orientational order, whereas translational cubic order only emerges in sufficiently large clusters of orientational order.

Despite its simplicity, the hard cube system clearly exhibits an intricate pathway to nucleation, suggesting that other anisotropic particle systems might show similarly complex kinetic behaviour.

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**#251 - Active Model H: Scalar Active Matter in a Momentum-Conserving Fluid**

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Recent theories predict phase separation among orientationally disordered active particles whose propulsion speed decreases rapidly enough with density. Coarse-grained models of this process show time-reversal symmetry (detailed balance) to be restored for uniform states, but broken by gradient terms; hence detailed-balance violation is strongly coupled to interfacial phenomena. To explore the subtle generic physics resulting from such coupling we introduce a phase-field model that minimally violates detailed balance via a leading-order square-gradient term and in which a scalar concentration field is coupled to a momentum-conserving solvent. We find that, in the so called “dry” systems (where there is no momentum conservation, such as in contact with a momentum-absorbing wall) the additional detailed-balance violation term has modest effects on coarsening dynamics, but alters the static phase diagram by creating a jump in (thermodynamic) pressure across flat interfaces. On the other hand, in “wet” systems (where momentum is conserved) activity creates a contribution to the deviatoric stress that causes a negative interfacial for contractile swimmers. We predict that domain growth ceases at a length scale where diffusive coarsening is balanced by active stretching of interfaces, and confirm this numerically.

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**#252 - Quantum walk of twisted photons***Lorenzo Marrucci (I) - Università di Napoli Federico II*

The angular momentum of a light beam in the paraxial limit can be split into spin and orbital components (SAM and OAM). Usually these components are independent of each other (in the paraxial limit), but a spin-orbit coupling can be obtained by means of suitable optical devices named *q-plates*. A *q-plate* is based on a space-variant birefringent medium, typically a liquid crystal, whose optic axis is azimuthally patterned in the transverse plane with a topological singularity of integer or semi-integer charge  $q$  at the center. A number of applications of these devices have been demonstrated in classical photonics and in quantum optics during the last few years.

In this talk, I will show how a sequence of *q-plates* combined with polarization optics can be used to carry out quantum-walk simulations in the OAM space of photons. Based on this idea, a new platform to carry out quantum simulations with photons travelling in a single free-space beam, without spatial interferometers, has been demonstrated [1]. This new platform allows one to study novel aspects of the quantum walk phenomena that are not so easily accessible with other approaches, including the system underlying band structure and the dynamics of delocalized quantum states [1].

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**#253 - Manipulating and Measuring Light at the Nanoscale***Peter Banzer (I) - Max Planck Institute for the Science of Light**Other Authors: Gerd Leuchs (Max Planck Institute for the Science of Light)*

Light can exhibit a very complex spatial structure. For instance when light gets highly confined or focused to dimensions on the order of the wavelength, the polarization, phase and intensity distributions may form three-dimensional field landscapes. Tailoring or manipulating the spatial structure of light at the nanoscale paves the way for an incredibly wide range of applications in the fields of super-resolution imaging and microscopy, nano-optics, plasmonics, quantum optics and material processing. In addition, highly confined light fields may also feature intriguing novel properties, such as counter-intuitive topologies, hidden in the complex field. However, measuring the fully vectorial distribution of the electromagnetic field of light at the nanoscale, including the amplitude and phase distributions of individual field components, is a sophisticated task. Available methods require complex near-field measurement systems and calibration techniques, or they lack the capability of measuring the full field information. Recently, we have introduced a nano-interferometric method, which is based on coherent nano-probing. This very versatile particle-based experimental approach in combination with a theoretical algorithm allows for the measurement of electric field distributions with nanometer spatial resolution. Furthermore, it enables both the characterization of optical systems as well as highly confined fields used as tools in the above-mentioned fields of research and the experimental study of novel electromagnetic phenomena hidden in complexly tailored light fields. Also the experimental study of purely evanescent nanoscale fields is possible with a recent extension of the theoretical algorithm. In this presentation, we want to introduce the basic concept of the aforementioned method and highlight recent experiments on the manipulation of light at the nanoscale.

**#254 - Manipulating CV quantum correlation by tailoring the environment noise***Alberto Porzio (I) - CNR - SPIN Napoli**Other Authors: Daniela Buono (Dipartimento di Ingegneria Industriale, Univ. di Salerno), Gaetano Nocerino (Trenitalia spa, DPR Campania, Ufficio di Ingegneria della Manutenzione, IMC Campi Flegrei, Napoli, Italy), Fabrizio Illuminati (CNSIM, INFN and Dipartimento di Ingegneria Industriale, Univ. di Salerno)*

The amount of quantum correlations owned by a pure quantum state is uniquely determined by the entanglement measure. Contrarily, for mixed quantum states, there is no a unique measure able to spill-out the correlation content of a bipartite unseparable state.

Quantum Discord, a class of geometric measures, is able to distil quantum from classical-like correlations. In particular, the Gaussian discord of response is related to the error probability of a quantum reading protocol [1].

In this contribution we show experimentally how the presence of noisy environment can enhance the quantum correlations strength in a bipartite continuous variable unseparable state. In particular we investigated the behaviour of a squeezed state by looking at its evolution in a Gaussian lossy channel where the lossy transmission mirrors the addition of thermal photon in the state generation Hamiltonian.

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**#255 - GLASS-BASED 1-D DIELECTRIC MICROCAVITIES***Alessandro Chiasera - IFN - CNR CSMFO Lab.*

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The development of optically confined structure is a major topic in both basic and applied physics including information engineering, biological and medical sciences, sensing. One-dimensional photonic crystals have been widely investigated and still remain an outstanding tool for new photonics, being the simplest system to exhibit a so-called photonic bandgap and therefore one of the easiest to handle in order to obtain tailored optical devices. RF sputtering techniques has demonstrated to be a viable technique for fabrication of 1D-photonic crystals allowing management and manipulation of the spectroscopic properties of optical and spectroscopic properties [1,2]. Here we will present recent results obtained by our consortium regarding: (i) 1D photonic crystals allowing  $\text{Er}^{3+}$  luminescence enhancement concerning the  $^4I_{13/2} \rightarrow ^4I_{15/2}$  transition; (ii) disordered 1D photonic structures that are very interesting for the modelization and realization of broad band filters and light harvesting devices; (iii) 1D microcavities, activated by a layer based on poly-laurylmethacrylate matrix containing  $\text{CdSe}@\text{Cd}_{0.5}\text{Zn}_{0.5}\text{S}$  quantum dots, leading to coherent emission.

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## #256 - Optically Controlled Elastic Microcavities

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Polymeric micro-photonic structures are particularly attractive for their high quality, low cost and versatility in integrated photonics devices. A reversible and stable tuning of the optical properties provides a higher level of functionality. We present the photo-induced tuning of a whispering gallery mode (WGM) microlaser obtained by employing a liquid crystal elastomers (LCE) actuator. Taking full advantage of the mechanical properties of this material, we demonstrate the possibility to opto-mechanically tune different polymeric integrated devices.

Polymeric microgoblet resonators [1], doped with a laser dye, are processed on a silicon substrate by electron beam lithography. Opto-mechanical control of the lasing frequency of the structure is obtained with a LCE microcylinder positioned in the center of the PMMA cavity. The cylinders are fabricated employing direct laser writing (DLW) on a LCE mixture kept in the nematic phase [2] with the uniaxial alignment parallel to the symmetric axis of the cylinder. The WGM resonator was pumped with a nanosecond pulsed laser at 532 nm with 1 kHz repetition rate, so that the lasing modes of the resonator can be excited and the LCE cylinder can be heated up exploiting the absorption of the thermal effect dye present in the LCE mixture. Once the LCE temperature overcomes the transition temperature, a phase transition from nematic to isotropic state is induced. As a result the molecules become disordered yielding an in-plane isotropic expansion of the microcylinder, which in turn expands the goblet changing its resonance wavelength. We report a continuous reversible resonance shift up to 2 nm of the lasing modes by varying the laser pump power [3].

Exploiting the 3D high resolution of the DLW lithographic technique, engineered LCE structures have been integrated in 3D polymeric micro-circuits constituted by WGM resonators coupled to single mode waveguides to achieve the optical dynamic tuning of their photonic properties.

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#### #257 - Laser coherence manipulation: narrow linewidth mid-infrared sources

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The demand of narrow-linewidth, metrological-grade laser sources is common to a variety of applications ranging from high-sensitivity spectroscopy to frequency metrology, remote sensing, cold atoms and molecules, communication technology. Here we summarize our recent achievements in the manipulation of the coherence properties of mid-infrared laser sources, by means of a variety of methods ranging from optical injection to all-electronic linewidth narrowing techniques (e.g. frequency locking to narrow resonances or phase locking to stable optical references). Preliminary results and perspectives of laser frequency stabilization to high-finesse whispering gallery mode microresonators will be discussed.

#### #258 - Light robot: Laser fabrication of liquid crystalline elastomer for photonic applications

Hao Zeng - LENS - European Laboratory for Non-Linear Spectroscopy

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Liquid crystalline elastomers (LCEs)<sup>1,2</sup> have been considered as one of the best candidate for artificial muscles, and have been used in creating bio-mimetic micro-robot. Recently developed Direct Laser Writing (DLW)<sup>3</sup> technique enables to fabricate 3D high-resolution LCE structures which can be actuated by light. This new concept allows for the realization of free-form microscopic actuators with multiple functionalities<sup>4</sup>. Applications can be foreseen in tunable photonics and light controlled robotics. Here, we introduce the first artificial walker<sup>5</sup> equipped with LCE micro-muscle. The walker is powered totally by light energy, smaller than any known living walking species, and capable of random or directional walking, rotating or jumping on different surfaces. These robots can be considered as a tiny platform to study different physics ruling on microscopic scale, and have the capacity of creating interactions between light and movement. One can even envision to embed the robots with a tiny piece of photonic structure as a photonic crystal or random laser.

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**#259 - GENERATION OF “STRONG SHOCKS” FOR THE SHOCK IGNITION APPROACH TO ICF**

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The contribution describes the results obtained in experiments performed on the “Shock Ignition” approach to ICF at the LULI and LIL (France), PALS (Czech Republic) and GEKKO (Japan) laser facilities, aimed at study the process of shock generation and the physics of laser-plasma interaction at intensities up to  $10^{16}$  W/cm<sup>2</sup>. In all experiments we used different laser beams or pulse shaping first to produce a pre-plasma and second to launch a strong shock.

The first goal of the experiments was to study the shock created at  $1\omega$  and at  $3\omega$  in order to demonstrate the generation of very large shock pressures. The second goal was to study the backscattering of light. We recorded spectra and measured the total reflected energy. The third goal was to study the production of supra-thermal electrons in order to investigate their possible contribution to the generation of the shock wave.

We measured the shock breakout time at the backside of the target with SOP and VISAR diagnostics, the back scattered light (SBS and SRS reflected energy), the plasma extension with interferometry, plasma temperature with X-ray spectroscopy, and the hot electrons with an X-ray imager.

At LULI and LIL we also studied shock dynamics in planar plastic targets as compared to “hemispherical” targets, The bigger laser energy and longer pulse duration available at LIL allowed to extend the study in conditions which are closer to a real ICF scenario (LIL is the prototype laser chain for LMJ).

Finally at LULI and GEKKO we used X-ray radiography as a diagnostics of shock dynamics. The shock front was studied at different times by changing the temporal delay between the beam producing the shock and a ps-backlighting beam producing a Kasource. In all cases, we compared the results with CHIC 2D simulations in order to infer the maximum pressure inside the target.

**#260 - Kinetic treatment of collisionless plasmas in non-symmetric configurations**

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The talk deals with the Vlasov-Maxwell theory recently established for the kinetic description of non-symmetric equilibria in collisionless magnetized astrophysical plasmas. The non-relativistic regime is treated first. Two different configurations are considered, respectively the case of spatially non-symmetric kinetic equilibria and the case of equilibria which do not exhibit a functional dependence on the single-particle energy (energy-independent equilibria). Solutions for the equilibrium kinetic distribution functions are explicitly constructed and expressed by generalized Gaussian distributions which depend on the relevant set of single-particle adiabatic invariants. In this reference, the role of the magnetic moment conservation predicted by gyrokinetic theory is discussed. Qualitative properties of these solutions are investigated, including the calculation of fluid fields and the investigation of the constraints posed by the Maxwell equations. Both the configurations are shown to exhibit a kinetic dynamo, whereby the equilibrium magnetic field can be self-generated by the equilibrium plasma currents. As a notable feature, energy-independent equilibria are proved to be generally non-neutral and characterized by the absence of the Debye screening effect, while admitting absolute stability criteria with respect to axisymmetric electromagnetic perturbations. Finally, the covariant formulation of the theory appropriate for the treatment of relativistic astrophysical plasmas in curved space-time is illustrated.

**#261 - Magnetic islands in the high plasma density regime on FTU**

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In tokamak fusion devices it is of great interest to operate at high plasma density, that is observed to be limited by the appearance of catastrophic events causing of plasma disruption [1]. The process usually considered to be the cause of the tokamak density limit is a radiation instability occurring when the radiation loss near the edge region overcomes the heat flux emerging from the core. This produces a contraction of the temperature profile, and accordingly a shrinkage of the current profile. As a result of the current profile change, a global MHD mode, such as the tearing mode, is driven unstable, leading to the density limit disruption. Dedicated density limit experiments were performed on the Frascati Tokamak Upgrade (FTU), exploring the high density domain in a wide range of values of plasma current and toroidal magnetic field [2, 3]. The development of large-amplitude tearing modes in proximity of the density limit on FTU shows a complex behaviour that can be outlined in three stages during the density ramp-up. First stage: the magnetic island grows smoothly at constant rotation frequency. Second stage: amplitude and frequency feature

large cycles of oscillations, with peak amplitude increasing progressively across cycles; in particular, the amplitude and frequency oscillations show a well defined phase portrait, determining a so called "limit cycle" on the amplitude/frequency plane [4]. Third stage: the island grows quickly to large amplitude and locks; this stage generally ends in a disruption. The main results of the performed experiments will be summarized. [1] M. Greenwald, *Plasma Phys. Control. Fusion* 44, R27-R80 (2002) [2] G. Pucella, O. Tudisco, et al., *Nucl. Fusion* 53, 083002 (2013) [3] G. Pucella, et al., *Proc. 40th EPS Conf. on Plasma Phys.*, P5.139 (2013) [4] G. Pucella, et al., *Proc. 42nd EPS Conf. on Plasma Phys.*, P4.112 (2015)

### #262 - Radiation transport effects on the electron energy distribution function under high speed flows for aerospace and astrophysical applications

Giuliano D'Ammando - CNR

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Radiation transport effects on the electron energy distribution function under high speed flows for aerospace and astrophysical applications

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A state-to-state (STS) kinetic model, coupling the master equations for internal distributions of heavy species with the Boltzmann equation for the free electrons and the radiative transfer equation (RTE) has been developed. Local plasma emissivity and absorption coefficient are calculated using an accurate model [1] taking into account bound-bound, bound-free and free-free transitions. Solution of the RTE is performed to determine self-consistent values for the rate coefficients of photoinduced atomic transitions and photoionization [2]. Rate coefficients of electron-impact processes are self-consistently calculated integrating the local non-equilibrium electron energy distribution function over the relevant cross section [3]. A detailed collisional-radiative model (CMR) of a  $H_2$ ,  $H_2^+$ ,  $H$ ,  $H^+$ ,  $He$ ,  $He^+$  and  $e^-$  plasma, including the most significant radiative, electron impact and heavy particle impact elementary processes, is applied to study the structure of a steady radiative shock created at the impact of an hypersonic vehicle ( $v=20-50$  km/s) with high-temperature Jupiter's atmosphere. The supersonic expansion of the plasma in an high enthalpy flow is also investigated, showing that the radiation model has a strong impact on the evolution of the distributions and internal temperatures generating large structures in the electron energy distribution functions [4,5]. Preliminary results concerning the application of this model to low density conditions of relevance in astrophysical shocked flows [6] are also reported.

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### #263 - 3D evolution of an externally injected electron beam in a plasma in the presence of a plasma wake field driven by an ultra-short electron bunch: hollow formation and stability analysis

Fatema Tanjia - Università di Napoli Federico II and INFN Sezione di Napoli

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A 3D evolution of an electron beam, externally injected in a plasma in the presence of a plasma wake field, is carried out. The wake is driven by an ultra-short relativistic axially-symmetric femtosecond electron bunch. Within the thermal wave model description, the spatiotemporal evolution of the beam is governed by a Schrodinger-like equation which accounts for both the plasma wake potential driven by the electron bunch and the self-interaction. The plasma wake potential driven by the bunch obeys to a Poisson-like equation which takes suitably into account the interplay between the sharpness and high energy of the bunch. It is shown that a channel through the beam is formed longitudinally. This seems to be a final stage of the 3D evolution of the beam which involves the appearance of small filaments and bubbles around the longitudinal axis. The bubbles coalesce forming a relatively stable axially-symmetric hollow beam structure.

### #264 - Macroscopic dynamics, topology and transport barrier formation in Reversed Field Pinch plasmas

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The reversed-field pinch configuration for the magnetic confinement of fusion plasmas is characterized by the emergence of self-organized quasi-helical states found both in magnetohydrodynamics (MHD) simulations and in high current RFP experiments. Numerical modeling can reproduce with high fidelity the MHD dynamics of high current RFP experiments, which are characterized by the formation of helical states, quasi-periodically relaxed to 3D states by strong reconnection events [1]. Seed helical perturbations at the magnetic boundary are expected to direct the plasma towards alternative helical states and first experimental tests have indeed confirmed this capability. Of particular interest is the possibility to stimulate non-resonant helical states, which feature better topological properties [2, 3]. Simulation results and first experimental evidence of alternative helical states formation in RFX-mod will be presented, together with a discussion of the different magnetic topology properties and their impact on transport barrier formation [4].

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## #265 - A transport beam-line solution to control optically accelerated proton beams

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Laser-target acceleration represents a very promising field for several potential applications, from the nuclear physics to the medical ones. However, some extreme features, not suitable for multidisciplinary applications, as a poor shot-to-shot reproducibility and a wide energy and angular distributions, characterize optically accelerated ion beams. Therefore, beyond the improvements at the laser-target interaction level, a lot of efforts have been recently devoted to the development of specific beam transport devices in order to obtain controlled and reproducible output beams.

In this framework, a three years contract has been signed between the INFN-LNS (IT) and ELI-Beamlines (CZ) to provide the design and the realization of a complete transport beam-line, named ELIMED, dedicated to transport, the diagnostics and dosimetry for laser-driven ion beams. The transport devices will be composed by a set of permanent quadrupoles able to collect, focus and pre-select in energy laser driven beams up to 60 MeV/u, and an energy selector system made of conventional resistive magnets. The in-air section will consist of ionization chambers, optimized for high dose-rate ion beam and of an innovative Faraday Cup, accurately designed to optimize the absolute dose measurement of high-pulsed ion beams. In this contribution an overview of the current status of design and development of the ELIMED beam-line along with a discussion of the adopted solution will be given. Moreover, some experimental results obtained with both transport and dosimetry prototypes, already realized at the INFN-LNS and tested both with conventional and laser-driven beams, will be presented.

## #266 - Inverse Faraday Effect driven by Radiation Friction

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In the interaction of extremely intense laser pulses with thick targets, as foreseen with next generation lasers such as ELI, radiation friction effects are expected to convert a major fraction of the laser energy into incoherent radiation. For a circularly polarized laser pulse, the radiative dissipation allows to absorb electromagnetic angular momentum, which in turn leads to the generation of an ultrastrong (Gigagauss) magnetic field. Such Inverse Faraday Effect driven by radiation friction is demonstrated and analyzed in three-dimensional simulations.

**#267 - Magnonic Crystals: controlling spin wave propagation on the nanoscale**

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Magnonic crystals (MCs) represent a new class of metamaterials with periodically modulated magnetic properties[1,2] where, similarly to light in photonic crystals,[3]the spin waves (SWs) dispersion is characterized by the presence of allowed magnonic states and ranges of forbidden frequencies.[4]The latter are related to the appearance of Brillouin Zones, induced by the artificial periodicity of the pattern geometry. MCs offer better prospects for miniaturization of a new generation of spin logic devices, filters, and waveguides operating in the GHz frequency range.[5]To this respect, knowledge of the magnonic band structure and of the physics underpinning the dispersion curves of magnonic modes is of paramount importance for any desired application.[6]In this presentation, recent results obtained by Brillouin light scattering for the SW band diagram of one and two-dimensional MCs consisting of arrays of identical elements (stripes and dots),[7,8]and antidot arrays where circular holes are drilled into a continuous ferromagnetic film,[9,10,11,12] are presented.

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**#268 - Dynamical properties of 2D ferromagnetic antidot lattices**

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The effects of the ground-state magnetization on the dynamical properties of a two dimensional (2D) magnonic crystals represented by an array of antidot lattices (ADLs) are theoretically studied. ADLs are composed of circular nanoholes of diameter  $d = 200$  nm, periodicity  $a = 610$  nm embedded into a CoFeB film having thickness of 41 nm [1]. The analysis of collective modes has been carried out by means of a micromagnetic method, named Dynamical Matrix Method (DMM). The mode propagation is studied starting from two different ground state magnetization: a) applying an external magnetic field  $H$  along the  $z$ -axis and the Bloch wave vector  $K$  parallel to the  $x$ -axis, b) placing  $H$  along the  $y$ -axis and  $K$  parallel to the  $x$ -axis. The aim of this study is to describe the dynamic properties in terms of effective quantities and to investigate the influence of the two different ground state magnetizations on the dispersion relations. From the inspection of spatial profiles of collective modes it is identified, for both the static magnetization configurations, an effective wavelength commensurable with the periodicity  $a$  of the system which is related to the Bloch wavelength. Correspondingly, it is defined an effective wave vector  $k$  linked to the Bloch wave vector. It is found that, independently of the magnetization ground-state studied, a simple relation between the effective quantities and the Bloch quantities holds. It is demonstrated that the Bloch rule depending on the Bloch wave vector can be derived from the effective rule involving the effective wave vector independently of the ground-state magnetization [2,3]. On the other hand, other two characteristic physical quantities typical of collective modes like the group velocity and the band width strictly depend on the ground-state magnetization. In particular, the group velocity is higher for in-plane magnetization than for out-plane magnetization, while the band width behavior is reversed. A discussion of the possible reasons at the basis of the different trend of these physical quantities is also carried on.

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**#269 - Ferroelectric control of magnetic anisotropy in CoFeB/BaTiO<sub>3</sub> heterostructures with perpendicular magnetic anisotropy***Lorenzo Baldrati - Dipartimento di Fisica, Politecnico di Milano**Other Authors: Christian Rinaldi (Dipartimento di Fisica, Politecnico di Milano), Marco Asa (Dipartimento di Fisica, Politecnico di Milano), Matteo Cantoni (Dipartimento di Fisica, Politecnico di Milano), Stefano Bertoli (Dipartimento di Fisica, Politecnico di Milano), Riccardo Bertacco (Dipartimento di Fisica, Politecnico di Milano)*

Electric control of magnetic properties has recently received great attention from both the technological and fundamental points of view: the electric flipping of the magnetization for instance allows to provide low-power switching in MRAMs.[1] Many efforts of the community were devoted to the study of multiferroic materials, since they provide a direct interplay between the electric and magnetic degrees of freedom. Magneto-electric coupling (MEC) in heterostructures made of ferroelectric and ferromagnetic materials is a promising route towards room-temperature electric-field-controlled memory and logic spintronic devices. We have already demonstrated the on-off switching of the ferromagnetism in the interfacial Fe layers of the Fe/BaTiO<sub>3</sub> (BTO) system, via an electric field applied across the BTO. [2,3] Here we present the demonstration of room temperature ferroelectric control of magnetic anisotropy and voltage-assisted magnetization flip in inorganic microcapacitors based on the prototypical CoFeB/BaTiO<sub>3</sub> interfacial multiferroic, at TTL compatible values ( $\pm 4V$ ).[4] Ta(2 nm)/ CoFeB(-1 nm)/ BTO(150 nm)/ La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub>(50 nm) multilayers were grown on SrTiO<sub>3</sub> (001) single crystal substrates by Pulsed Laser Deposition and Magnetron Sputtering. Perpendicular magnetic anisotropy of the CoFeB layer was obtained below a CoFeB thickness of 1.3 nm, after magnetic field annealing. Microcapacitors (100x70 microns) were patterned on the stack in a top-top configuration by means of optical lithography and ion beam etching. LSMO serves as a conducting and lattice matching layer while Ta is used for capping and stabilization of the out-of-plane anisotropy of the CoFeB layer. We performed a complete magnetic and ferroelectric characterization by Vibrating Sample Magnetometry, micro-Kerr, Positive Up Negative Down and Dynamic Hysteresis Measurement techniques. We found a magnetic coercive field variation up to 60% versus voltage applied to BTO, and we attributed this variation to purely electronic effects related to ferroelectric polarization. Noteworthy, we were able to flip the magnetization from downwards to upwards and vice versa by reversing the voltage polarity across the BTO in a magnetic bias field of  $\pm 2.8$  mT. Reversing this uniform low bias field and addressing each pad via voltage pulses, allows to reversibly switch the magnetization of individual spintronic devices in a chip.

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**#270 - Asymmetries arise when a ferromagnet meets a heavy metal***Paolo Moras - Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, 34149 Trieste, Italy**Other Authors: Gustav Bihlmayer (Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany), Polina Sheverdyaeva (Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, 34149 Trieste, Italy), Sanjoy Mahatha (Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, 34149 Trieste, Italy), Marco Papagno (Dipartimento di Fisica, Università della Calabria, 87036 Arcavacata di Rende (Cs), Italy and Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, 34149 Trieste, Italy), Jaime Sánchez-Barriga (Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Straße 15, 12489 Berlin, Germany), Oliver Rader (Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Straße 15, 12489 Berlin, Germany), Luka Novinec (Materials Research Laboratory, University of Nova Gorica, Vipavska 13, 5000 Nova Gorica, Slovenia), Sandra Gardonio (Materials Research Laboratory, University of Nova Gorica, Vipavska 13, 5000 Nova Gorica, Slovenia), Carlo Carbone (Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, 34149 Trieste, Italy)*

We observe asymmetric electron band dispersion in ferromagnetic cobalt films grown on a heavy metal tungsten crystal, in apparent contrast to electron band behavior in centro-symmetric solids. Theoretical analysis ascribes these effects to the large exchange and Rashba spin-orbit fields, that characterize the two materials and combine at their interface. The recent discovery of current-induced magnetization reversal in ferromagnetic/heavy metal bilayers represents one of the most promising novelties in the field of spintronics. The mechanism beneath this phenomenon is currently under debate. In the present work we examine the fundamental interactions that define the electronic structure of ferromagnetic/heavy metal junctions. As a model system we consider ferromagnetic cobalt films on a tungsten support. The discrete and spin-polarized bands of the cobalt films display strong asymmetries in the band dispersion along structurally equivalent directions, which fully reverse upon switching the magnetization. Experimental and theoretical evidence shows how high exchange and high Rashba spin-orbit interactions of different materials can be combined at an interface. A component of the Rashba field is added to the exchange field, leading to a dependence of the electronic bands on the magnetization direction. These results give new and direct insights for the understanding of the microscopic origin of spin-orbit-induced magnetization reversal effects.

**#271 - Collective nature of spin excitations in superconducting cuprates probed by resonant inelastic x-ray scattering***Matteo Minola - Max Planck Institute for Solid State Research**Other Authors: Greta Dellea (CNISM, CNR-SPIN and Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy), Hlynur Gretarsson (Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany), Ying-Ying Peng (CNISM, CNR-SPIN and Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy), Yi Lu (Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany), Juan Porras (Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany), Toshinao Loew (Max-*

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In recent years resonant inelastic x-ray scattering (RIXS) showed that high- $T_c$  superconducting cuprates [1-3] exhibit damped but well defined spin-excitations (*paramagnons*) at all dopings, with dispersions and spectral weights closely similar to those of magnons in undoped cuprates, even far away from the antiferromagnetically ordered state, where  $T_c$  vanishes and electrons behave as in a Fermi Liquid. These observations are rather counter-intuitive: magnon-like excitations indeed are expected to damp heavily - and eventually to vanish - when entering the Stoner particle-hole continuum. On the other hand, individual excitations of this continuum (*including spin-flip excitations*) are expected to grow with doping, and eventually to become the dominant excitations in the Fermi Liquid regime. The debate involves also theoretical results: recent state-of-the-art numerical work [4] showed that magnons can indeed persist up to rather high doping but, on the other hand, explicit calculations of the RIXS cross-section of the particle-hole excitations [5] suggested that all Cu- $L_3$  RIXS results could be interpreted in terms of band structure effects. In order to solve this controversy, we used RIXS, for the first time also with the analysis of the scattered photon polarization, to understand the nature of dispersive spin excitations in the high temperature superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  over a wide range of dopings ( $0.1 \leq x \leq 1$ ) [6]. We monitored the excitation profiles as the incident photon energy was detuned away from the resonant condition, and we found that the spin excitations energy is independent of detuning for all doping levels up to the optimal one. These findings demonstrate that the largest fraction of the spin-flip RIXS profiles in doped cuprates arises from magnetic collective modes, rather than from incoherent particle-hole excitations as suggested in Ref. [5]. On the other hand, preliminary measurements on a highly overdoped  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+x}$  suggest that band structure effects may play a crucial role deep inside the Fermi Liquid regime. I will discuss the experimental findings and their implications for the theoretical description of the electron system in the cuprates.

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## #272 - Structural flux closure transitions in magnetic filaments

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Magnetic colloids tend to assemble into linear chains with a head-to-tail alignment of their dipole moments. This assembly is favored by external magnetic fields and/or relatively strong dipole-dipole interactions. The formation of such chains and their behavior is a key factor in the properties of magnetic fluids and magnetic soft matter systems, like magnetic gels and filaments. In the latter system, the chains of magnetic colloids are stabilized by permanently crosslinking the colloids with polymers, forming supramolecular semiflexible polymer-like chains.

In diluted dispersions of both free magnetic colloids and filaments under low entropy conditions, the dipolar chains tend to not remain open, rather they form closed rings that add an extra dipolar bond and close the magnetic flux inside the cluster. These rings are responsible of the non monotonic magnetic response of ferrofluids at low temperatures. As the concentration of the system increases and the intrachain interactions become dominant, the isolated ring-shaped chains are replaced by aggregates with different branching points, up to the limit of forming a single percolating network.

In this contribution we study the flux closure structural transitions that take place in systems of magnetic filaments with decreasing temperature, and analyze the difference brought by the permanent links with respect to dispersions of free colloids. We combine extensive Langevin dynamics simulations with analytical models based on density functional theory and network analysis. We pay a special attention to the determination of the characteristic temperature at which the closure occurs as a function of the chain length and linking mechanism for the case of a single chain, and compare the results to those for the filament gas.

## #273 - Towards room temperature IrMn/MgO-based antiferromagnetic memories: investigation of the MgO influence on the IrMn properties

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Memory elements based on antiferromagnets (AF) deserve large interest because of their high packaging density and robustness versus external perturbations. In a previous work [1] we demonstrate that in Ta/MgO/IrMn(2.5 nm) tunnelling junctions, grown on SrTiO<sub>3</sub> substrates, two distinct metastable resistance states can be set by field cooling the heterostructures from above the Néel temperature (-170 K) with the external magnetic field along different orientations. Tunneling Anisotropic Magnetoresistance (TAMR) [2] up to 10% at 120 K upon field cooling along the in-plane or out-of-plane direction provided the first demonstration of an electrically readable magnetic memory device, in which the information is stored within the AF active layer.

Two key steps towards the diffusion of this technology are 1) extending the operation of the device to room temperature and 2) moving to silicon. To this scope, we investigated by Vibrating Sample Magnetometry the temperature dependence of the exchange bias and magnetic coercive field of CoFeB thin layers embedded in Si/SiO<sub>2</sub>//CoFeB/IrMn(*t*)/MgO/Ru structures. We found that, for IrMn thickness (*t*) smaller than 6 nm, the presence of MgO suppresses the exchange bias, while it is present for Ru capping down to 2.5 nm. Instead, from *t*=6 nm the exchange bias is present even with MgO capping, with a blocking temperature of about 180 °C, largely allowing for room temperature operation of the device.

In order to clarify the role of MgO in inhibiting exchange bias below 6 nm of IrMn, we investigated by photoemission spectroscopy the effect of the MgO or Ru capping on the IrMn (oxidation, stoichiometry, band alignment, etc.) and we end up with the realization of IrMn/MgO/Ru tunnel junctions to understand the feasibility of TAMR at room temperature.

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#### **#274 - Slow relaxation of the magnetization in an Isostructural series of Zinc-Lanthanide complexes: an integrated EPR and AC susceptibility study**

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Lanthanide based molecular complexes have shown potential to behave as single molecule magnets proficient to function above cryogenic temperatures. In this work we explore the dynamics of one such family, [Zn(LH)<sub>2</sub>Ln](NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O- (Ln = Nd<sup>3+</sup>, Dy<sup>3+</sup>, Tb<sup>3+</sup>, Ho<sup>3+</sup>, Er<sup>3+</sup>, Yb<sup>3+</sup>, where LH is the monoanion of a dicompartmental Schiff base ligand derived from 2-formyl-6-hydroxymethyl-p-cresol and 1,3-diamino-2-propanol). The series has a single lanthanide ion as a magnetic center in a low symmetry environment; the energy landscape, magnetic properties and dynamics of the series is explored using X-band EPR, DC and AC magnetic susceptibility techniques over a range of temperature, field and frequency. DC magnetic data show  $\chi T$  values consistent with expected single ion values. Yb<sup>3+</sup>, Nd<sup>3+</sup> and Er<sup>3+</sup> derivative show EPR spectra typical for easy-axis and easy-plane respectively. No peaks in the out-of-phase susceptibility measurements are observed even in an external applied field for the complexes. However, Dy<sup>3+</sup> derivative show slow relaxation of the magnetization both in zero and applied field up to 30 K and is EPR silent. Magnetization versus applied field measurements of the Dy<sup>3+</sup> derivative at 2 K reveal a butterfly hysteresis which tends to close with increase in temperature, thus confirming single molecule magnet behavior in DyZn<sub>2</sub> complex. Dynamic susceptibility measurements as a function of increasing field show more than one peak in the out-of-phase susceptibility data, thus indicating that relaxation in the DyZn<sub>2</sub> complex is governed by multiple processes, like Direct, Raman and Orbach processes, which we investigated in detail.



**#275 - Nanoscale YBCO devices to look at the microscopic mechanism of high critical temperature superconductivity***Floriana Lombardi (I) - Chalmers University of Technology**Other Authors: R. Arpaia, R. Baghdadi, M. Arzeo, T. Bauch Quantum Device Physics Laboratory, Mc2, Chalmers University of Technology, SE-41296, Göteborg, Sweden*

The phase diagram of the high-T<sub>c</sub> cuprate superconductors (HTS) is shaped by the spontaneous emergence of various ordered states, tuned by doping and driven by the many competing degree of freedom, where not only charge and spin are of relevance, but also lattice and orbitals have an active role in building up the ground state. The identification of all ordered states is crucial for understanding high-temperature superconductivity. In strongly correlated systems, the tendency of the valence electrons to segregate in periodically modulated structures can lead to the formation of a peculiar charge order. The evidences for a new charge state, ubiquitous in all cuprates families and with translational/rotational symmetrybreaking have recently come from major developments of synchrotron based X-ray scattering. However, while X-ray scattering experiments have clearly shown that the charge order competes with superconductivity, the consequences of such a local arrangements of charge carriers on the transport properties of HTS devices remain to be seen.

In this contribution I will review our recent experiments on HTS nanoscale devices showing how they can be decisive to get new insights into the microscopic mechanism leading to superconductivity in these materials.

I report on our progress in realizing a novel spectroscopic technique, based on an YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub>(YBCO) underdoped nanoisland, that allows an unprecedented energy resolution, thanks to Coulomb blockade effects, a regime practically inaccessible up to now in these materials. An all YBCO Single Electron Transistor (SET) has been fabricated by using biepitaxial grain boundaries as tunnel barriers. In such a devices we find that the energy required to add an extra electron to a nanometer size YBCO island depends on the parity (odd/even) of the excess electrons on the island itself and increases with magnetic field. This is inconsistent with a pure  $d_{x^2-y^2}$ -wave symmetry and demonstrates a complex order parameter component on the island that needs to be incorporated into any theoretical model of HTS. I will also present unconventional transport properties in YBCO nanowires. We have been able to engineer pristine YBCO nanowires, with cross sections as small as 40×50 nm<sup>2</sup>, retaining the full superconductive properties with record values for the critical current density  $J_c$ . Starting from untwinned thin YBCO films grown on MgO (110) close to the optimally doped regime, nanowires of the same length but different width, have been patterned at different angles. Preliminary measurements of the critical current density have revealed an unconventional  $J_c$  angular dependence for nanowire's width below a certain threshold ( $w \approx 80$  nm), that cannot be accounted for by considering the anisotropy of the London penetration depth along a and b YBCO axis.

**#276 - Superconductors for future accelerators***Amalia Ballarino (I) - CERN*

After the discovery of the Higgs boson and the completion of the Standard Model, future accelerator facilities, which will help in understanding some of the still unanswered questions of fundamental physics, are under study. While operation and exploitation of the LHC will continue until about 2035, with an upgrade in luminosity planned in 2023, higher-energy colliders are proposed as powerful tools that will address some of the outstanding questions of particle physics. These colliders are based on high-field (16 T-20 T) magnets, which will need superconductors with performance well above that of today state-of-the-art materials. A review of the potential of Low Temperature Superconductors and High Temperature Superconductors for future accelerator facilities is presented, with a focus on performance of the presently available materials and on the needs for further development.

**#277 - Superconducting cables: an enabling technology for nuclear fusion reactors***Luigi Muzzi (I) - Superconductivity Laboratory, ENEA*

The application of superconducting materials in large magnets for plasma confinement has been identified as a key aspect of nuclear fusion reactors since the early stage of their development. Superconducting magnets are now recognized as an enabling technology for fusion machines based on magnetic confinement, due to the large size and to the long pulse duration required. The main experiment in the field, ITER (International Thermonuclear Experimental Reactor), currently under construction in southern France as a worldwide collaboration of seven partners (EU, China, India, Japan, US, Russia and South Korea), makes extensive use of Nb-based, low temperature superconductors. Within this frame, the design of large size – high current Cable-in-Conduit conductors (CICC) based on the mature technology of Nb<sub>3</sub>Sn and NbTi multi-filamentary wires, has been greatly optimized in the last decade, also thanks to the improved comprehension of structural behavior and transport phenomena at microscopic scale. The state-of-the-art of CICC technology, well represented by the ITER conductors, will be illustrated; the optimization margins to be envisaged will be discussed, together with possible prospects of solutions based on High Temperature Superconducting (HTS) materials.

**#278 - Vortex-Antivortex coexistence in Nb based Superconductor/Ferromagnet heterostructures***Domenico D'Agostino - University of Salerno*

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We used low temperature Magnetic Force Microscopy to investigate the vortex dynamics in Superconductor/Ferromagnet (S/F) heterostructures realized by Py/Nb thin films. By tuning the magnetic state of the ferromagnet new physical phenomena can be observed due to the interaction between the Abrikosov vortex lattice in the Nb layer and the periodic, stripe-like, Py magnetic domains. The analysis of the different behaviors of these systems is of great importance for applications, allowing to predict and control the electronic properties of the S/F hybrids. In our samples Nb thickness ( $d$ ) varied in the range 100–360 nm and Py thickness ( $d_p$ ) in the range 1–4  $\mu\text{m}$ . To ensure that the F and S layers were only magnetically coupled a 10 nm  $\text{SiO}_2$  was deposited on top of the Py film. The behavior above and below the Nb superconducting critical temperature was analyzed by means of a cryogenic Scanning Force Microscope.

Low temperature MFM allowed us to collect topographic and magnetic force maps in the same area of the sample at different tip-sample heights varying in the range of 50–280 nm. We used commercial Si cantilevers with magnetic coating, resonance frequency  $f_0$  of about 75 kHz, magnetic moment  $0.3 \times 10^{-16} \text{ Am}^2$  and coercivity  $< 3 \times 10^4 \text{ A/m}$ . Before measuring the tip was magnetized in the upward direction. In our experiments a variety of different behaviors were observed [1-3], depending on the intensity of the out of plane magnetization component  $M_0$  of the Py layer as well as on the interrelations among some "geometrical" parameters of the hybrids, i.e., the Nb penetration depth  $\lambda$  and thickness  $d$  and the Py stripe half period width  $w$ . When  $w > \lambda$ , in zero external applied field, depending on  $d$ , the samples showed "spontaneous" Vortices-Antivortices (V-AV) formation in a chain-like configuration along the magnetic stripes due to the alternating out of plane component  $M_0$  of the Py stray field. We have analyzed the observed experimental results within a theoretical model which deals with  $M_0$  intensity threshold, causing spontaneous V-AV formation [4], finding the estimates  $M_0 > 17 \text{ G}$  for the Py-4  $\mu\text{m}$ ,  $M_0 > 21 \text{ G}$  for the Py-2  $\mu\text{m}$  and, finally,  $15 \text{ G} < M_0 < 25 \text{ G}$  for the Py-1  $\mu\text{m}$  [5].

[1] M.Iavarone et al. IEEE Magnetics Society 48, 11 (2012)

[2] A.M. Cucolo et al., Journal of Superconductivity and Novel Magnetism, 25, 2167-2171 (2012)

[3] M.Iavarone, et al. Phys. Rev. B 84, 024506 (2011)

[4] R. Laiho, et al, Phys. Rev. B 67, 144522 (2003)

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## #279 - Sine-Gordon breathers in long Josephson junctions

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The formation of breathers in a properly excited long Josephson junctions (LJJ) is computationally investigated. The features of a LJJ are related to the behavior of the *order parameter*  $\varphi$ , that is the phase difference between the macroscopic wave functions describing the superconducting condensate in the two electrodes. The dynamics of  $\varphi$  is described by a nonlinear partial differential equation, the well-known *sine-Gordon* (SG) equation, in this work used including a damping term and an applied bias current. The SG equation admits plasma waves and several traveling wave solutions, that is *solitons*, i.e. *kink* and *antikink*, and stationary or moving *breathers*. In particular, a breather is a bound kink/antikink pair oscillating with an internal frequency and decaying in time. Several theoretical and computational studies about breathers in LJJ exists, despite of the lack of experimental works devoted to their detection. The experimental observation of breathers in LJJ is nowadays a challenge and many impediments exist. Indeed, a breather has to efficiently generated and entrapped and, moreover, it doesn't manifest itself as clear mean voltage difference or magnetic flux through the junction. This work is devoted to establish an experimental setting to produce breathers in a LJJ. The study is based on the phenomenon called the *nonlinear supratransmission* (NLS). Due to the nonlinearity of the medium, that is the junction, energy transmission can also occur exciting the system using a signal with a frequency in ranges usually forbidden. In our model, one end of the junction is sinusoidally driven by a pulse of amplitude  $A$  and frequency  $\omega$  lower than the JJ plasma frequency. A 2D parameters space  $(A, \omega)$  is split in two areas, one with the absence of NLS, that is without energy flowing into the system, and another in which every combinations of SG solutions are generated and propagate along the junction. Finally, in correspondence of specific  $(A, \omega)$  values, the creation of only breathers comes to light. The analysis is enhanced modifying the damping parameter, the duration of the external pulse and the applied bias current. The robustness of the generated breathers is evaluated including a Gaussian noise source into the "perturbed" SG model. Therefore, we compute the percentage of surviving breathers as a function of the noise intensity and how their lifetime is affected by the thermal fluctuations.

**#280 - An experimental approach to observe energy spectrum in superconducting film with periodic hole arrays**

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The problem of electrons under the influence of a two-dimensional periodic potential (Bloch electrons) and a uniform applied magnetic field was studied theoretically three decades ago by Hofstadter<sup>1</sup>, who obtained a fractal energy spectrum composed of sub-bands and mini-gaps called the Hofstadter butterfly. However, experimental verification of the Hofstadter butterfly has been hindered by the fact that the magnetic field required to study the physics related to the Hofstadter butterfly of Bloch electrons in a crystalline lattice would be several hundred Tesla which is not accessible experimentally. Here, we report that, an applied magnetic field and superconducting thin films perforated with periodic hole (anti-dot) arrays in the superconducting state, we have discovered an approach capable of revealing the characteristics of the Hofstadter butterfly. We demonstrate that when the parameters such as the diameter and the period of the hole array are carefully chosen, several characteristics of the Hofstadter butterfly can be observed. Our approach opens a way to study the Hofstadter butterfly and related physics using conventional laboratory facilities.

**#281 - Flux-Flow Instability in Mesoscopic Superconductors**

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Conventional and quantum superconducting electronics are based on micro- and nano-scaled devices often operating in the so-called mesoscopic regime. In this regime, superconductors exhibit peculiar phenomena intimately connected to their intrinsic properties.

Flux-Flow Instability (FFI) is the name used to classify a group of phenomena related to different fundamental mechanisms (mostly electronic or thermal) connected to quasiparticle energy relaxation processes. Regardless of the mechanisms, in terms of Current-Voltage Characteristic (CVC) a unique feature is observed, i.e. an abrupt jump from the flux-flow branch to the normal state. A critical value for the velocity of the Abrikosov vortex lattice is associated to the point in the CVC where the jump is observed, namely the instability point.

In this work we investigate the so far totally unexplored interplay between mesoscopic regime and FFI. Here we present experimental data showing how such confinement can strongly influence the FFI behaviour as a function of the applied magnetic field. These experimental findings are supported by simulation based on Time-Dependent Ginzburg-Landau model. We find that flux-flow motion is limited by reaching an upper threshold of the vortex critical velocity at low fields.

**#282 - Topological spin-triplet superconductors: interface to magnets and edge states***Mario Cuoco (I) - CNR-SPIN and Dipartimento di Fisica, Università di Salerno**Other Authors: CNR-SPIN and Dipartimento di Fisica, Università di Salerno*

The past decades have been marked by a growing interest in the study of the interplay between superconductivity and magnetism in heterostructures, both for the potential applicative impact and the underlying fundamental phenomena. The physical properties of heterostructures are strongly interrelated to the nature of the interface and its electronic states at the cross-talk region. A special position in the variety of electronic states is taken by gapless modes at the boundary of materials whose bulk is gapped and owe their existence on the global symmetries of the bulk state without depending on the details of the surface scattering and other sample-dependent parameters. Simple band insulators or superconductors do not support robust low-energy states at the boundary. The topological non-trivial nature of the bulk state and the bulk-boundary correspondence theorem are fundamental aspects that determine the existence of surface states. Within the superconducting systems, a notable class of superconductors with non-trivial topological number is the two-dimensional (p+i p)-wave superconductor with time reversal symmetry breaking, which has in the single layered SrRuO compound its leading candidate. The rapid growth of interest in this areas has also led to the proposal of an additional class of spin-triplet superconductors with time reversal invariance, that contrary to the chiral ones can have zero modes that come in pairs and can support counterpropagating edge states of opposite spins near the boundary that carry a spin-current. In this talk we analyze the emergent phenomena that occur at the boundary of chiral and helical spin-triplet superconductors and at the interface with a magneti system. We discuss the basic mechanisms that enter in the coupling between magnetism and superconductivity at the interface and the important consequences on the electronic edges states and the spin/charge electronic transport.

This work has been done in collaboration with:

P. Gentile, C. Noce, and A. Romano, CNR-SPIN and Dipartimento di Fisica, Università di Salerno, Fisciano, Italy

D. Terrade and D. Manske, MPI Stuttgart, Stuttgart, Germany

I. Vekhter, University of Louisiana, Baton Rouge, USA

P. Brydon, University of Maryland, College Park, USA

**#283 - Subgap spectrum of normal-superconductor nanowire junctions: helical regime and Majorana bound states from exceptional points***Ramon Aguado (I) - Consejo Superior de Investigaciones Científicas (CSIC)*

The linear conductance through a helical region, such as a depleted semiconducting nanowire with strong Rashba spin-orbit coupling and in the presence of a Zeeman field, is expected to exhibit a reentrant behavior with a helical gap of half-quantum conductance [1]. If one takes into account the finite length of the depleted section, this ideal scenario changes and the conductance acquires superimposed Fabry-Perot oscillations [2,3]. These normal transport features translate into distinct subgap states when the leads become superconducting (i.e. in a SNS junction geometry). In particular, Fabry-Perot resonances within the helical gap become zero-energy crossings, well below the critical field  $B_c$  at which the superconducting leads become topological. As a function of Zeeman field or Fermi energy, these crossings form characteristic loops and evolve continuously into Majorana bound states as the Zeeman field exceeds  $B_c$ . As I will argue, this characteristic loop pattern could be used to unambiguously identify the helical regime in nanowires [3].

Interestingly, when a helical normal region becomes a long contact in a NS geometry, the junction may host Majorana states well below  $B_c$  (namely with  $S$  in the trivial regime) after crossing an 'exceptional point' in parameter space, defined as a degeneracy in the complex eigenvalues of the effective non-Hermitian Hamiltonian of the NS junction. The Majorana character of these states, derived from the eigenvalue bifurcation at the exceptional point, is protected by particle-hole symmetry and is not a result of fine tuning while their finite lifetime can be tuned to arbitrarily large values as the junction approaches perfect Andreev reflection. I will show how exceptional-point Majoranas exhibit the full range of properties associated to conventional closed-system Majorana bound states, while not requiring topological superconductivity [4].

[1] P. Streda and P. Seba, PRL, 90, 256601 (2003).

[2] D. Rainis and D. Loss, PRB, 90, 235415 (2014).

[3] J. Cayao, E. Prada, P. San-Jose and R. Aguado, PRB 91, 024514 (2015)

[4] P. San-Jose, J. Cayao, E. Prada, and R. Aguado, arXiv:1409:7306

**#284 - Dirac single particle and plasmon excitations in topological insulators***Stefano Lupi (I) - Department of Physics, Sapienza University*

Topological Insulators (TIs), like Bi<sub>2</sub>Se<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub>, are one of the most intriguing issues at focus in Condensed Matter Physics. TIs exhibit a band gap in the bulk like ordinary insulators, but have intrinsic 2D conducting states on their edge and surface. This means that the topology, associated with the electronic wavefunctions of the system, changes discontinuously when passing from the bulk

to the surface. The edge states arise from a strong spin-orbit coupling, and they are backscattering protected, i.e. not sensitive to disorder (except that coming from magnetic impurities). Such as graphene, TIs surface charge transport is carried out by Dirac fermions, with a very high surface carrier density ( $n \geq 10^{13} \text{ cm}^{-2}$ ), compared to typical values on metal surfaces. Apart single particle excitations, Dirac fermions in TIs sustain exotic plasmonic (collective) modes whose properties of tunability and temperature dependence can be used for photonics applications at the nanoscale. Moreover, unlike plasmons in metals, Dirac plasmons in TIs are expected to be strongly affected by an external magnetic field  $B$  due to fact that the cyclotron frequency is comparable to the the plasmon frequency, in particular when plasmons are engineered in the terahertz region of the electromagnetic spectrum.

In this talk, after a general review on the properties of Topological Insulators, I will discuss the terahertz linear response of Dirac plasmons in TIs and their behavior under a strong magnetic field up to 30 T. The appearance of strong non-linear optical effects, when the THz electric field reaches values on the order of 1 MV/cm, will be also discussed.

Both the linear and nonlinear experiments provide a unifying picture of single particle and collective electronic excitations in Topological Insulators.

#### #285 - Fractional charge spectroscopy and non-equilibrium effects in topological protected edge states

*Alessandro Braggio - CNR-SPIN*

We investigate how to extract information on the fractional quantum hall phases by investigating the response of a resonant circuit coupled to quantum point contact kept at extremely low temperatures[1]. This setup is a sort of spectroscopic tool of the different fractional excitations that not trivially populate the quantum hall phase. After we apply some of the developed concept in order to investigate the non-equilibrium physics in the topological protected edge modes of a topological insulator and how to detect them [2]. The general formalism discussed would be in general applicable also to quantum Hall systems showing the non-trivial role of interactions in the edge dynamics.

[1] D. Ferraro, M. Carrega, A. Braggio and M. Sassetti "Multiple quasiparticle Hall spectroscopy investigated with a resonant detector" *New J. Phys.* 16, 043018 (2014)

[2] M. Carrega, I. Levkivskiy, N. Magnoli and A. Braggio, work in progress

#### #286 - Adsorption of organic and metallorganic molecules on Bismuth Selenide: investigating the robustness of surface states

*Marco Caputo - Laboratoire de Physique des Solides - Université Paris-Sud*

*Other Authors: Simone Lisi (Dipartimento di Fisica - Università di Roma La Sapienza), Mirko Panighel (ICN2-Institut Catala de Nanociencia i Nanotecnologia), Lama Khalil (Laboratoire de Physique des Solides - Université Paris-Sud), Giovanni Di Santo (Laboratory Micro & Nano Carbon Consorzio INSTM UdR Trieste-ST c/o ELETTRA - Sincrotrone Trieste S.C.p.A.), Evangelis Papalazarou (Laboratoire de Physique des Solides - Université Paris-Sud), Andrzej Hruban (Institute of Electronic Materials Technology), Marchin Konczykowski (Laboratoire des Solides Irradiés, CNRS-UMR 7642 & CEA-DSM-IRAMIS, Ecole Polytechnique), Ivana Vobornik (Istituto Officina dei Materiali (IOM)-CNR, Laboratorio TASC), Jun Fuji (Istituto Officina dei Materiali (IOM)-CNR, Laboratorio TASC), Andrea Goldoni (Laboratory Micro & Nano Carbon Consorzio INSTM UdR Trieste-ST c/o ELETTRA - Sincrotrone Trieste S.C.p.A.), Marino Marsi (Laboratoire de Physique des Solides - Université Paris-Sud)*

Topological insulators constitute a new class of materials that is attracting the attention of scientific community in the latest years. While semiconductor in the bulk, 3D topological insulators ( $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  among the others) possess surface states crossing the Fermi level protected by time-reversal symmetry. Strong spin-orbit coupling characteristic of such heavy elements locks the spin to the momentum, forbidding backscattering for electrons occupying their surface states. All these features make Topological insulators an ideal candidate in the field of spintronics.

Organic molecules have demonstrated their potential in the same field. Molecular-based spin valves have already been realized, while metallophthalocyanines (MPc) paved the way for the so-called molecular magnetism. New physics can arise by the interaction of metalorganic molecules and topological insulators, with completely new perspectives in the field of spintronics.

Here we show results from an Angle Resolved Photoemission Spectroscopy (ARPES) study of the prototypical Cobalt Phthalocyanine (CoPc)/ $\text{Bi}_2\text{Se}_3$  and Metal-free Phthalocyanine (2HPc)/ $\text{Bi}_2\text{Se}_3$  interfaces. Special care will be devoted to the different modification of the surface states induced by the adsorption of the metalorganic and the metal-free molecules.

#### #287 - Interaction effects in nonequilibrium transport properties of a four-terminal topological corner junction

*Francesco Romeo - University of Salerno*

*Other Authors: Roberta Citro, (Dipartimento di Fisica "E. R. Caianiello", University of Salerno, Italy)*

We study the transport properties of a four-terminal corner junction made by etching a two-dimensional topological insulator to form a quantum point contact (QPC) [1]. The QPC geometry enables interboundary tunneling processes allowing for the coupling among states with different helicity, while the tight confinement in the QPC region activates charging effects leading to the Coulomb-blockade physics. Peculiar signatures of these effects are theoretically investigated using a scattering field theory modified to take into account the electron-electron interaction within a self-consistent mean field approach. The current-voltage characteristics and the current fluctuations (noise) are derived beyond the linear response regime. Universal aspects of the thermal noise of the corner junction made of helical matter are also discussed.

[1] F. Romeo and R. Citro, Phys. Rev. B 90, 155408 (2014) and references therein.

### #288 - Spin fractionalization in topological insulators

*Alessio Calzona - Università di Genova, Dipartimento di Fisica*

*Other Authors: Matteo Carrega (CNR-SPIN), Giacomo Dolcetto (CNR-SPIN), Maura Sassetti (Dipartimento di Fisica Genova)*

The interacting helical edge states of two-dimensional topological insulators represent a new paradigm of the one-dimensional world, where peculiar quantum phenomena can be investigated. Motivated by recent experiments on charge fractionalization, we theoretically analyze and propose a setup, based on a topological insulator platform, that allows to observe the fractionalization of the spin degree of freedom. An electron wavepacket injected from one metallic lead into an interacting helical region splits into charge and spin fractional excitations. By inducing spin-charge separation, the two degrees of freedom can be decoupled, and thus independently investigated by time-resolved electrical measurements. Moreover, this device allows the detection of single neutral excitations with fractionalized spin only via electrical probes.

### #289 - Electronic structure and topological states in curved nanostructures

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The past few years have been characterized by increasing theoretical and experimental efforts aiming at the identification of new classes of materials with non-trivial topological properties. The example of topological insulators have taught that spin-orbit coupling is usually a key ingredient to generate topological phases. This requirement largely restricts the number of potential candidates materials. Within this context, an appealing perspective comes from recent predictions [1] about the possibility to induce via geometric strain, or equivalently via geometric curvature, a sizeable Rashba spin-orbit interaction in materials that intrinsically do not possess an appreciable spin-orbit coupling. From this concept it follows that the palette of possible materials where non-trivial topological states may emerge can be drastically enlarged through the geometric manipulation of conventional materials. The feasibility of novel curved nanoarchitectures looks very promising, especially in consideration of the recent great experimental advances in the synthesis of complex three-dimensional nanostructures with curved geometries. These systems represent an excellent example of solid-state platforms where to investigate novel quantum effects rising because of the influence of space curvature on the physical properties of quantum objects. Within this context we have analyzed the specific features of the electronic structures characterizing curved nanostructures as a function of the geometric curvature, also investigating the conditions for the possible emergence of topological states.

[1] P. Gentile, M. Cuoco, C. Ortix, SPIN, Vol. 3, No. 2 (2013) 1340002

**#290 - Solitons, bifurcation and bistability with beams of light in nematic soft matter**

Gaetano Assanto (I) - Tampere University of Technology and Univ. Roma Tre

Other Authors: A. Piccardi (U. Roma Tre), A. Alberucci (Tampere Univ. technology)

Light self-localization in liquid reorientational media such as nematic liquid crystals supports the formation of spatial optical solitons. These nonlocal solitons are stable and robust in the presence of perturbations, collisions, interactions [1]. When the optic axis of the uniaxial medium is orthogonal to the electric field of the propagating light beam, the nonlinear optical response features an abrupt change versus excitation and a power threshold, the so called optical Fredericks transition, with a nonlinear bifurcation via symmetry breaking. Optical wavepackets and inherent noise, in fact, can alter the initial symmetry and turn into self-trapped beams with opposite transverse velocities. We demonstrate that such system can give rise to optical bistability versus input power, with hysteretic switching between soliton and diffractive states of the beam [2].

[1] M. Peccianti and G. Assanto, "Nematicons", *Phys. Rep.* 516, 147-208 (2012).

[2] N. Kravets, A. Piccardi, A. Alberucci, A. Buchnev, M. Kaczmarek and G. Assanto, "Bistable self-trapping with optical beams in a reorientational medium", *Phys. Rev. Lett.* 113, 023901 (2014).

**#291 - Meta-Molecules for nonlinear nano-photonics**

Joseph Zyss (I) - University

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The ongoing field of molecular engineering for nonlinear optics is aiming at improving the performances of organic molecules and polymers, from the definition of optimized molecular templates, to their assembly into functional materials and devices. However fruitful per se, this approach does not fill the 20 to 400 nanometers gap, in-between point-like molecules and the wavelength dimension, with its potential to connect micro- to nano-photonics and bring photonics at a par with electronics. In the wake of nanotechnologies and nano-photonics, this gap came to be increasingly occupied over the past decade by nonlinear plasmonics, entailing both new physics and applications of major interest [1]. Over recent years, the concept of "meta-molecules" has emerged in this field, based on relevant associations of "meta-atomic" building blocks in the form of either metallic nano-cavities or nanoparticles, enabled by advanced "top-down" technological tools including e-beams, ion beams and semiconductor based wet etching technologies. In parallel, nonlinear optics developed a new branch in multiphoton microscopy, allowing to perform detailed investigations down to unprecedented scales, with polarization resolved second-harmonic generation confocal microscopy (2) has a forefront tool. At the upstream conceptual end, the design of nanostructures remains driven by fundamental symmetry considerations, now implemented in the different frame of localized and propagative plasmon excitations [2-5], that require more elaborate models to account for non-local excitations extending over a fraction of the wavelength and more.

We will review some recent developments in this fast evolving domain [6-8], including the various enabling fabrication technologies, the relevance of symmetry lowering considerations and a number of experimental advances confronted to theoretical models, which have all contributed to the emergence of nonlinear meta-structures as relevant building blocks for nonlinear photonics. Future work will be addressing hybrid nano-architectures tailored towards nano-biophotonics applications and consisting of metallic nano-patterns decorated by functional molecules.

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**#292 - Geometric origin of rogue solitons in optical fibres**

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Nondeterministic giant waves, denoted as rogue, killer, monster, or freak waves, have been reported in many different branches of physics. Their physical interpretation is however still debated: despite massive numerical and experimental evidence, a solid explanation for their spontaneous formation has not been identified yet. Here we propose that rogue waves [more precisely, rogue solitons (RSs)] in optical fibers may actually result from a complex dynamical process very similar to well-known mechanisms such as glass transitions and protein folding. We describe how the interaction among optical solitons produces an energy landscape in a highly dimensional parameter space with multiple quasi-equilibrium points. These configurations have the same statistical distribution of the observed rogue events and are explored during the light dynamics due to soliton collisions, with inelastic mechanisms enhancing the process. Slightly different initial conditions lead to very different dynamics in this complex geometry; a RS turns out to stem from one particularly deep quasi-equilibrium point of the energy landscape in which the system may be transiently trapped during evolution. This explanation will prove to be fruitful to the vast community interested in freak waves.

### **#293 - Microwave generation by nonlinear crystals irradiated with a high-power, 1064 nm, mode-locked laser**

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We report a new technique to produce microwave (MW) in the cm band, in which nonlinear crystals are irradiated with a high-power, near-infrared (IR), mode-locked laser.

Typically, microwave are produced by optical heterodyning techniques, in which the superposition of two adjacent laser lines in a nonlinear crystal leads to a beat at the difference frequency that lies in the microwave domain.

By contrast, we have devised a new technique [1], in which a high-intensity mode-locked laser at 1064 nm induces the second order dielectric response of nonlinear crystals such as potassium orthotantalophosphate, and others. The laser delivers trains of 2000, 10-ps short, optical pulses at a repetition rate in the GHz domain. The phenomenon of optical rectification gives origin of a time-dependent polarization of the crystals at a frequency determined by the repetition rate of the laser.

We have studied the emitted WM radiation by enclosing the crystals either in a MW cavity that acts as a selective filter or in a waveguide that is a broad band receiver. By investigating the relationship between laser intensity and MW amplitude we have demonstrated that the generation of MW is due to the second order nonlinearity of the crystal polarization that is also responsible for the generation of the second harmonic.

We have also investigated the effect of the tensor nature of the second order nonlinear dielectric susceptibility by studying how the MW production depends on the orientation of the plane of laser light polarization with respect to the crystallographic axis of the crystals.

We have also shown that the present phenomenon can be used to realize an inline, ultrafast monitor of the quality of a mode-locked IR laser because the crystal dielectric response at optical frequencies is due only to electrons and does not have any ionic contribution. Moreover, such crystals are transparent in the near IR range and a laser can pass through them without losing any appreciable amount of energy [2].

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### **#294 - Sub-kHz-linewidth mid-infrared optical parametric oscillator**

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Highly stable and spectrally pure laser sources are crucial for a wide range of demanding applications, including frequency metrology, precision tests of fundamental physics, and high-resolution spectroscopy in the mid-infrared region of the electromagnetic spectrum, where intense ro-vibrational transitions of many molecules are present. Among the mid-infrared sources, OPOs combine in the same device unique features, such as high power, single mode emission, tunability and wide spectral coverage, thus proving their suitability for high-sensitivity spectroscopy. A large number of visible and near infrared lasers have been narrowed down to sub-Hertz-linewidth and their frequency absolutely stabilized up to the level of the best optical frequency standards, while sub-kHz narrowing of mid-infrared sources is limited to a couple of gas lasers and more recently to quantum cascade lasers. Here, we report on sub-kHz linewidth narrowing of an optical parametric oscillator (OPO) idler mode.



**#295 - Frequency comb generation in nonlinear media**

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Optical frequency combs, originally conceived for frequency metrology, are nowadays routinely used in a wide range of scientific and technological applications. Ultrafast mode-locked lasers, first used for comb generation, have then been joined by continuously-pumped Kerr microresonators, exploiting the third-order nonlinearity of the materials, and by quantum cascade lasers. Materials with second-order susceptibility,  $\chi(2)$ , have been used for transferring otherwise generated OFCs to different spectral regions. We experimentally demonstrate frequency comb generation in a continuously-pumped cavity-enhanced second-harmonic generation (SHG) system, where multiple, cascaded  $\chi(2)$  nonlinear processes enable the onset of broadband  $\chi(2)$ -comb emission, both around the fundamental pump frequency and its second harmonic. Our system shows a striking similarity with generation and dynamics of frequency combs in Kerr microresonators, as confirmed by a simple three-wave theoretical model we developed and extended to a general number of comb modes. This analogy unveils the possibility to predict and observe most of the effects occurring in Kerr-medium-filled cavities, such as multistable regimes, temporal solitons, FWM amplification, intermodal phase coherence and mode-locking, pulsed emission, etc., paving the way for a novel class of highly efficient and versatile frequency comb synthesizers based on second-order nonlinear materials.

**#296 - Irreversible quantum mechanics in nonlocal nonlinear optics**

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We review one of our recent theoretical and experimental developments on the simulation of fundamental physical models by nonlocal nonlinear optics. Specifically, we consider dispersive shock waves which dominate wave-breaking phenomena in Hamiltonian systems. In the absence of loss, these highly irregular and disordered waves are potentially reversible. However, no experimental evidence has been given about the possibility of inverting their dynamics and turn them into a regular wave-front. Nevertheless, the opposite scenario, i.e., a smooth wave generating turbulent dynamics is well studied and observed in experiments. Here we introduce a new theoretical formulation for the dynamics in a highly nonlocal and defocusing medium described by the nonlinear Schroedinger equation, showing that a defocusing medium realizes the optical analog of a reversed harmonic oscillator in the highly nonlocal regime. It has been shown [A. R. Bohm, R. Scurek, and S. Wikramasekara, "Resonances, Gamow Vectors and Time Asymmetric Quantum Theory," (1999), arXiv:nucl-th/9902076v1 [nucl-th]; A. R. Bohm, J. Math. Phys. 22 (1981); D. Chruscinski, Open Sys. Information Dyn. 9, 207221 (2002), arXiv:math-ph/0206009v1 [math-ph]] that this theoretical model is the paradigm for irreversibility and can describe dissipative systems where no time-symmetry holds.

Our theory is based on the concept of Gamow vectors, that are commonly adopted in the Rigged Hilbert Space formulation of irreversible quantum mechanics. This nonlinear vectors are a power dependent generalizations of the counter-intuitive and heretofore elusive exponentially decaying states in Hamiltonian systems. We show that nonlinear Gamow vectors play a fundamental role in nonlinear Schroedinger models: they may be used as a generalized basis for describing the dynamics of the shock waves, and affect the degree of irreversibility of wave-breaking phenomena. Gamow vectors allow to analytically calculate the amount of breaking of time-reversal with a quantitative agreement with numerical solutions.

We also report on the experimental observation of these states, characterized by a quantized decay rate, generated by an optical photothermal nonlinearity [S. Gentilini, N. Ghofraniha, E. DelRe, and C. Conti, Phys. Rev. A 87, 053811 (2013)].

**#297 - Optomechanics of random and nonlinear media**

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We report on a theoretical investigation on the effect of randomness and nonlinearity on optical forces. We find that disorder enhances the light-induced mechanical effects and that ultra-fast nonlinear polarization may give a negative contribution to the optical pressure.

The Balazs block (BB) furnishes a simple way for understanding the origin of optical pressure in terms of photon momentum exchange at the interface between a dielectric block and the surrounding medium. Albeit this analysis is oversimplified and hides a variety of fundamental problems, BB gives simple insights on optical pressure,  $p$ , and suggests that a possible way to take into account both disorder and nonlinear effects is through the total transmission  $T(\lambda)$ .

Several recent investigations show that light propagation and amplification in disordered matter can be controlled, and this possibility allows several applications. However, there is a specific field in which the benefits of randomness has not yet been

investigated, and that is optomechanics. Even if, from the perspective of optically activated nano-structured devices, understanding opto-mechanical forces (OMFs) due to many interfaces and to the related multiple scattering of light is pivotal.

Because of the small values of the OMFs, we solve the fully vectorial Maxwell equations within few-microns-sized systems made of disordered assemblies of dielectric nano-particles by means finite-difference-time-domain (FDTD) numerical simulations. By combining the calculus of the OMFs and the analysis of the light transport regime of ultra-short light pulses, we find that with increasing disorder the transverse components of the OMFs statistically broaden, correspondingly the diffusion constant and the transport mean free path decrease, and the optical pressure reaches a maximum. This maximum demonstrates that the momentum transferred to a disordered micron-sized composite object increases when approaching the localization regime. These findings open the road to the exploitation of photon random walk to determine the light-induced pressure for several micro-devices.

Another important effect that can affect the optical pressure emerging from a transparent material if irradiated by a laser beam is the ultra-fast optical nonlinearity. However, the effect of nonlinearity on optical pressure is often overlooked, even if a nonlinear optical effect may potentially be employed in many applications, such as optical manipulations, biophysics, optical tractor, and is relevant in fundamental problems such as the Abraham-Minkowsky dilemma. We theoretically show that an ultra-fast nonlinear polarization of Kerr type can give rise to a negative contribution to the optical pressure, whose estimated order of magnitude is such as to be observable by measuring the deflection of a graphene membrane.

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**#298 - Silicon nanostructures for optoelectronic and photovoltaic applications: first-principle results**

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In recent years particular attention has been devoted to Silicon (Si) nanocrystals and nanowires, a powerful class of nanostructures which is opening substantial opportunities for optoelectronics and photovoltaics. These nanostructures are zero- and one-dimensional materials with diameter from few to some tenths of nanometers. They present unique size dependent electronic, optical and transport properties that are intrinsically associated with their low dimensionality and quantum confinement effect. In the recent years we have performed several ab-initio calculations in the framework of the Density Functional Theory and the Many-Body Perturbation Theory for free and matrix embedded Si nanocrystals and for Si and Ge nanowires. Among the different results we will concentrate here on Si nanocrystals. We will evaluate, in particular, effects induced by doping and co-doping on transport, optical and electronic properties of Si nanocrystals embedded in different matrices or passivated by H- or OH- groups. Moreover, we will investigate carrier multiplication dynamics in systems of isolated and interacting H-terminated Si nanocrystals. Effects induced by nanocrystals interplay on carrier multiplication processes will be analyzed.

**#299 - Whispering gallery microresonators to give a new twist to silicon photonics**

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Internet boom can be slowed down by power hungry data centers. Silicon photonics is the technology to face this. A new twist to silicon photonics is provided by microresonators which enable complex functions and devices. Microrings show different properties that can be integrated into functional silicon photonic devices. Single, coupled or cascaded microring geometries can be used to achieve complex functions. Still many aspects of the physics of photon confinement in small optical cavities have to be investigated. Therefore silicon microresonators are ideal devices for looking at new phenomena and new physics. Here we review and summarize few of these.

Specifically, within the European project SYMPHONY, we are developing a biosensor to detect aflatoxin in milk. We want to investigate Microresonators photonic structures with different dimensions and materials in order to figure out which one has the best performances. These are based on PECVD SiON and SiO<sub>2</sub>. Since we aim at a full integration in silicon, the photonic sensing unit operates in the near infrared (~850 nm) where suitable silicon photodetectors are available.

Another example is the coupling between a physical system and its environment which is known to activate new channels through which the system may dissipate energy. Along this, the coupling may induce a shift of energy levels of the system. In atomic context, the manifestation of these phenomena are described through well-known examples of the Coherent Population Trapping for decay channels and the electronic Lamb shift of electronic states of the Hydrogen atom.

**#300 - Interacting plasmonic nanostructures for nanophotonics and nonlinear optics applications**

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The capability to control light-matter interaction at the nanoscale is one of the main challenges in nanophotonics. To this aim, an efficient strategy is to exploit plasmonic effects (coherent oscillations of conduction electrons) in noble metal nanostructures. The coupling of light to surface plasmons in metallic nanostructures with tailored shapes and/or composition induces intense enhancements of the local electromagnetic field at the nanostructures, which can be further increased by exploiting the interaction among the plasmonic nano-building blocks. These properties are of great interest for nanophotonics and nonlinear optics applications since they can be effectively exploited to design plasmonic nanosystems with tunable and amplified nonlinear optical response and to control the quantum efficiency of emitters properly placed in close proximity to the plasmonic nanostructures. In this presentation, we will report on the results of our recent experimental investigation on the properties of some peculiar kinds of interacting plasmonic nanostructures synthesized by nanosphere lithography (NSL), that is, triangular nanoprism arrays (NPA), semi-nanoshell arrays (SNSA) and nanohole arrays (NHA). The plasmonic properties have been also theoretically investigated in the framework of a finite element model (FEM) electrodynamic approach. The results proved that the intense local-field enhancements occurring in these nanosystems give rise to a significant boost of their nonlinear optical response, activating phenomena otherwise not accessible in the intensity range that has to be employed to investigate the response of these materials without damaging the matrix. Moreover, particularly for the NHA configuration, the interaction with optical emitters (Er<sup>3+</sup> ions) at specific distance allows to get a high control over the radiative properties of the emitters both in terms of the decay rate and of the emission pattern, and a strong enhancement of the Er<sup>3+</sup> radiative efficiency in far-field is obtained with very modest losses in the plasmonic layer.

**#301 - Single-dot spectroscopy of silicon nanocrystals: ultranarrow linewidth and Auger biexciton recombination**

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The photoluminescence of silicon nanocrystals (Si-NCs) was studied using single-dot spectroscopy at different temperatures and for different host matrices. Ultranarrow homogeneous linewidths (resolution-limited, ~200 ueV) were detected at low temperatures (10 K) for NCs encapsulated in a very thin oxide shell, while broader lines were measured for particles with thicker passivation layers. This effect can be explained in terms of low-energy acoustic phonon modes, whose energies and coupling strengths depend on the surrounding medium. In addition, power-dependence measurements performed on narrow-linewidth Si-NCs revealed PL saturation at high excitations with no clear evidence of biexciton emission lines, suggesting dominant Auger recombination. However, single-dot time-resolved measurements allowed detection of the biexciton emission as a fast (~ns) initial transient under stronger excitation in the PL decay curve (~μs). The extracted Auger lifetimes, much shorter than the expected biexciton radiative decay times, seem to vary from dot-to-dot. Finally, the obtained temperature dependence of the biexciton quantum yield, not exceeding 0.1% below 10 K, provided explanation of the lack of specific lines in the low-temperature spectra of single Si-NCs.

**#302 - Optimization of plasmonic back reflector for broadband light trapping in thin-film solar cells**

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Light trapping is an attractive solution to increase the optical path length of sunlight in thin-film solar cells in order to improve their efficiency [1]. Among various structures proposed in literature, subwavelength noble-metal nanoparticles (NPs) have attracted significant attention due to their pronounced scattering properties at the localized surface plasmon resonance (LSPR), with the theoretical possibility of exceeding the theoretical  $4n^2$  limit, also known as the Yablonovitch limit [2].

Enhanced photocurrent in thin film solar cells has been demonstrated by placing the NPs on the rear side of the cell, forming what is known as a plasmonic back reflector (PBR) [3,4]. In such configuration, the NPs embedded in the Transparent Conductive Oxide (TCO) layer, which commonly separates the back mirror from the absorber, interact only with light that is not absorbed during the first pass through the cell material. The morphology of the NPs has a strong impact on the optical properties of the PBRs and can be tuned by an appropriate selection of the fabrication conditions [5]. High annealing temperature and long annealing time of the 12 nm thick precursor Ag film favor the formation of uniform NPs, in terms of size and shape. This results in desirable improvements of their optical response, namely increase of diffused reflectance, reduction of parasitic absorption and slight blue-shift of the resonance peak. By considering the average diffuse reflectance in the spectral range of interest, we address the optimization of PBR structures for a broadband light trapping in photovoltaic applications.

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**#303 - Enhanced second harmonic generation from multiresonant plasmonic nano-structures**

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Second Harmonic Generation (SHG) is well known to be a powerful imaging tool for background-free and non-damaging live tissues investigation. Field enhancements in plasmonic nanostructures are often exploited to effectively compensate for the lack of phase-matching in confined volumes with the aim of obtaining brighter nanoscale nonlinear probes. Recently, nanoantenna designs featuring a double resonance at both the excitation and the emission wavelengths have been proposed to improve SHG [1]. However, the high degree of symmetry in plasmonic materials at the atomic scale and in nanoantenna designs have so far poor

SHG efficiency [2]. We have circumvented these limitations and engineered gold single-crystalline nanoantennas working in the near-infrared that show unprecedented SHG efficiency thanks to (i) a multi-resonant response occurring at both the excitation and SH wavelength, (ii) a significant spatial overlap of the localized fields at the wavelengths of interest and (iii) a broken-symmetry geometry to achieve dipole-allowed SHG [3]. The effective combination of these key features in a single plasmonic antenna, characterized by the absence of local defects, allows optimizing SHG efficiency in a well-controlled fashion.

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### #304 - Genetically designed L3 photonic crystal cavities with measured quality factor exceeding one million

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Photonic crystal (PhC) cavities are becoming a leading approach in modern integrated nanophotonics due to their ability to confine light in small mode volumes ( $V$ ) for long times (i.e., with large quality factors ( $Q$ )). One of the key goals in research is to develop cavities that can reach ultra-high  $Q/V$  ratio with a high degree of integration. We will present the experimental realization of an optimized 2D PhC L3 nanocavity that features  $Q_s$  above  $10^6$  while maintaining a very small footprint.

Starting from the basic L3 cavity design, the guided-mode expansion (GME) method has been exploited for the optimization, combined with a genetic algorithm to explore the entire parameter-space [1,2]. This procedure enabled the determination of the optimal design with a computed maximum  $Q$ -factor of  $Q_{th}=5 \times 10^6$  at  $\lambda=1550$  nm. According to the new design, cavities have been fabricated in commercially available silicon on insulator (SOI) wafers, with additional support structures to suppress the buckling of the PhC silicon membrane. Then optical characterization of the fundamental cavity mode resonance has been performed, by cross-polarization resonant scattering spectroscopy [4]. A 10 MHz resolution tunable laser was used to excite resonantly the cavity mode, and the light scattered by the cavity was collected vertically in far-field with a  $NA=0.9$  objective. Thanks to the cross-polarization setting, we have precise control over the extinction of the reflected laser light and the linear polarized response of the cavity mode can be easily detected. Laser wavelength calibration is controlled through the fringes of a Fabry-Pérot interferometer with known free spectral range. The highest  $Q$ -factor measured is  $Q_{exp}=1.96 \times 10^6$  [4], 20 times larger than the highest  $Q$  previously reported on L3 cavities. The other nominally identical cavities on the same chip all displayed a clear resonance, with  $Q_s$  lying systematically in the  $1 \times 10^6$  range. We will also present new experimental insight into the effect of disorder and absorption on the statistical distribution of measured  $Q_s$ .

These genetically optimized PhC cavities are highly promising building blocks for integrated photonics applications, including silicon photonics, on-chip scalable platforms for quantum state control, and cavity optomechanics.

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# October 1

<b>Biophysical Models I</b>	<b>Cristian Micheletti</b>
Correlated electrons and cold atoms	Alberto Parola
<b>Imaging and non-destructive analysis</b>	<b>Austin Nevin</b>
New physics with ultrashort light and x-ray pulses I	Riccardo Cucini
<b>Quantum Optics and Coherent Manipulation</b>	<b>Benedetto Militello</b>
Organic on Substrates I	Alberto Verdini
<b>Gas Sensors and Biosensors for Health and Wealth</b>	<b>Giorgio Sberveglieri</b>
Advanced Optical Materials I	Marco Cannas
<b>Electronic and optical properties of low dimensional systems I</b>	<b>Stefano Roddaro</b>
Soft Matter I	Francesco Sciortino
<b>Advanced materials for energy applications I</b>	<b>Andrea Goldoni</b>
<b>Biophysical Models II</b>	<b>Cristian Micheletti</b>
Transport and anomalous dynamics	Andrea Gabrielli
Molecular liquids in equilibrium and non-equilibrium regimes	Franz Saija
<b>Geophysics</b>	<b>Alessandro Aiuppa</b>
New physics with ultrashort light and x-ray pulses II	Giacomo Ghiringhelli
<b>Quantum thermodynamics and quantum technologies 1</b>	<b>Massimo Palma</b>
Organic on Substrates II	Andrea Goldoni
<b>Nanomaterials and Nanotechnology: carbon nanotubes</b>	<b>Luigi Sangaletti</b>
Advanced Optical Materials II	Simonpietro Agnello
<b>Electronic and optical properties of low dimensional systems II</b>	<b>Stefan Huen</b>
Soft Matter II	Achille Giacometti
<b>Advanced materials for energy applications II</b>	<b>Marcella Bonchio</b>

**#305 - The complex structure of chromatin**

*Guido Tiana (I) - Department of Physics, University of Milano and INFN*

*Other Authors: Luca Giorgetti (Friedrich Miescher Institute, Basel) Edith Heard (Institut Curie, Paris)*

Chromatin is the whole DNA chain bound to proteins and RNA in the cellular nucleus. It is believed that the biological role of chromatin is not only that of packing DNA in a small volume, but also that of controlling gene expression, resulting in an epigenetic control on the cell. Recently, a class of experimental techniques were used to obtain contact maps of chromatin on the length scale of few kilobases; these contact maps are structured in blocks, suggesting that the chromatin fibre is assembled in small globules. Making use of polymer theory and of computer simulations based on the available experimental data, we investigate the conformational properties of the chromatin chain, trying to relate them to the activity of the associated genes.

**#306 - How chaperones assist the life of proteins: pulling, unfolding and Maxwell's demons**

*Paolo De Los Rios (I) - Ecole Polytechnique Fédérale de Lausanne*

Chaperone proteins are crucial for the maintenance of protein homeostasis in the cell. Among the several classes of chaperones that have been identified, Hsp70s stand out because in the course of evolution they have taken up a host of constitutive roles, besides the more traditional stress related ones.

Here we will review the present understanding of the mechanism of function of Hsp70 proteins in protein translocation and in protein folding, discussing how they relate to the modern description of non-equilibrium biochemical cycles.

**#307 - Stretching response of knotted and unknotted chains**

*Michele Caraglio - Università di Padova, Dipartimento di Fisica e Astronomia "Galileo Galilei"*

*Other Authors: Cristian Micheletti (SISSA, International School for Advanced Studies), Enzo Orlandini (Università di Padova, Dipartimento di Fisica e Astronomia "Galileo Galilei")*

Knots arise spontaneously in polymers that are sufficiently long or densely packed, and hence are ubiquitous in biopolymers where these conditions are met *in vivo*.

In recent years, the advent of more and more powerful single molecule manipulation and imaging techniques enabled direct measurements of mechanical and dynamical properties of knotted polymers and knots can even be artificially introduced into biopolymers such as actin filaments and linear DNA. The presence of knots is now known to affect the physical and functional properties of the hosting chain and, in principle, such differences in the behavior of knotted and unknotted chains can be exploited to detect the presence of knots in single biomolecules without the need of using single molecule imaging techniques, which are notoriously challenging.

Here we investigate, through molecular dynamics simulations, how and to what extent, the presence of knots can be inferred from a chain response to mechanical stretching. To this aim the behavior of tensioned knotted chains has been characterized in the whole range of pulling forces and compared to the behavior of unknotted chains.

We find that the stretching response has a very significant and non-trivial dependence on chain topology at low forces. In particular, the extension of knotted chains, normalised to unknotted ones, has a non-monotonic behaviour as a function of the applied tension. This notable feature is more pronounced when the complexity of the knot increases and could be exploited in force spectroscopy measurements to detect knots types in both flexible and semi-flexible chains.

**#308 - An efficient algorithm to perform local concerted movements of a chain molecule.**

*Stefano Zamuner - SISSA - Group: "Molecular and Statistical Biophysics"*

*Other Authors: Alex Rodriguez (SISSA, Trieste) Flavio Seno (Dipartimento di Fisica e Astronomia G. Galilei, Università degli Studi di Padova) Antonio Trovato (Dipartimento di Fisica e Astronomia G. Galilei, Università degli Studi di Padova)*

The devising of efficient concerted rotation moves that modify only selected local portions of chain molecules is a long studied problem. Possible applications range from speeding the uncorrelated sampling of polymeric dense systems to loop reconstruction and structure refinement in protein modelling. The efficiency of the methodology capitalizes on the inherent geometrical structure of the manifold defined by all chain configurations compatible with the fixed degrees of freedom. The chain portion to be moved is first opened along a direction chosen in the tangent space to the manifold, and then closed in the orthogonal space. As a consequence, in Monte Carlo simulations detailed balance is easily enforced without the need of using Jacobian re-weighting. Moreover, the relative fluctuations of the degrees of freedom involved in the move can be easily tuned. We show different applications: the manifold of possible configurations is explored in a very efficient way for a protein fragment and for a cyclic molecule; the "local backbone volume", related to the volume spanned by the manifold, reproduces the mobility profile of all- $\alpha$ ; helical proteins; the refinement

of small protein fragments with different secondary structures is addressed. The presented results suggest our methodology as a valuable exploration and sampling tool in the context of bio-molecular simulations.

### #309 - The structure of protein polymers, revealed by HPLC-SAXS experiments

*Vincenzo Martorana - National Research Council of Italy, Institute of Biophysics*

*Other Authors: Vincenzo Martorana,1 James Irving,2 Sarah V. Faull,3 Matteo Levantino,4 Imran Haq,1 Samuele Raccosta,1 Loredana Randazzo,1 Rosina Noto,1 David A. Lomas,2 Mauro Manno1 1. Inst. of Biophysics, Natl. Res. Council of Italy, via Ugo La Malfa 153, 90146 Palermo, Italy; 2. Wolfson Institute for Biomedical Research, U.C.L., London, UK; 3. Cambridge Institute for Medical Research, Cambridge University, UK; 4. Dept. of Physics and Chemistry, University of Palermo, Palermo, Italy.*

Serpinopathies are genetic diseases related to the deficiency of a serpin (SERin Protease Inhibitor) and/or its accumulation as polymer chain. The formation of protein polymers can also be triggered in solutions of a wild-type serpin by mild thermal stress. The first model for the serpin polymer formation, involving the insertion of the solvent exposed reactive loop of molecule A into the central beta-sheet of molecule B, has been recently challenged by two different crystallographic structures showing a varying degree of domain-swapping. In a series of experiments we measured the SAXS patterns of samples of alpha1-antitrypsin (AAT) purified from plasma, incubated for short times at 55 °C. The X-rays scattering was measured just after the passage through a chromatographic column that performs a partial separation of the polymers of different lengths. Furthermore, data obtained from SAXS experiments are known to be difficult to interpret when the systems are not homogeneous. To extract valuable information on the structure of AAT polymers we devised a model based on a collection of low resolution rigid monomer particles. Polydispersity was easily taken into account, thus allowing the fitting of the entire set of partially separated polymer populations at once.

### #310 - Volume exclusion effects in detailed balance systems

*Claudia Cianci - University of Edinburgh*

*Other Authors: Ramon Grima, Stephen Smith University of Edinburgh*

It is well known that the cell is a crowded environment and that many of the biochemical reagents exist in very low concentrations. Both of these facts increase the relevance of stochastic modelling. The accepted stochastic model of reactions on this scale is the Chemical Master Equation (CME), or Reaction Diffusion Master Equation (RDME) when spatial effects must be considered. In this paper, we show that the RDME reduces to the CME for detailed balance systems, and proceed to investigate how volume exclusion effects can alter the CME solution. We particularly focus on the crowding-induced changes that occur to the Fano factor, the coefficient of variation, and the skewness of the resulting distributions. We will consider two general classes of chemical systems, with and without chemical conservation laws. For each class of systems we will treat a specific example and we will verify our analytical results with simulation data obtained with the Stochastic Simulation Algorithm (SSA).

### #311 - The role of the antibody conformation in the formation of encounter complexes with small antigens

*Marta Galanti - Università degli Studi di Firenze, Dipartimento di Fisica e Astronomia and INFN*

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Antibodies are large, extremely flexible molecules, whose internal dynamics is certainly the key to their astounding ability to bind antigens of all sizes, from

small hormones to giant viruses. In this work, we build a shape-based coarse-grained model of IgG molecules and show that it can be used to generate 3D conformations in agreement with single-molecule Cryo-ET data. Furthermore, we elaborate a theoretical model that can be solved to any desired accuracy to compute the binding rate constant of a small antigen to an IgG in a prescribed 3D conformation.

Our model shows that the antigen binding process is tightly related to the internal dynamics of the IgG. We find that such link is more complex the more important are non-specific interactions with sites far from the paratopes. Our findings pave the way for further investigations of the subtle connection between the dynamics and the function of large, flexible multi-valent molecular machines.

### #312 - Design of Proteins and Biopolymers in explicit water: a Coarse-Grain Approach

*Valentino Bianco - University of Vienna, Faculty of Physics, Computational Physics*

*Other Authors: Ivan Coluzza, University of Vienna, Faculty of Physics, Computational Physics*

Protein/bio-polymer design concerns the "optimization" of a sequence of residues, given an alphabet of monomers, that folds in a target structure.

We present a new approach, based on a combination of water-protein coarse-grain model able, for a wide range of temperatures and pressures, to deeply explore the configurational space of a water-protein solutions. Accounting for the influence of protein



interfaces on the thermodynamic properties of the hydration shell, we show how the design of specific target structures is affected by the solvent properties. In turn, we show how the folding properties for different sequences, designed at different thermodynamic conditions, change.

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**#313 - A unified theoretical framework for cuprates, pnictides and fullerenes***Massimo Capone (I) - International School for Advanced Studies (SISSA) and CNR-IOM*

The link between high-temperature superconductivity and the physics of strong correlations has been forged by an immense number of studies of the copper-based superconductors (cuprates) in which a robust d-wave superconducting state emerges doping an antiferromagnetic Mott insulator. In this talk I will discuss the generality of this paradigm by demonstrating the role of Mott physics in the iron-based superconductors and in alkali-metal doped fullerenes.

For the iron-based superconductors, I will not argue that the *metallic* parent compounds (LaFeOAs, BaFe<sub>2</sub>As<sub>2</sub>, ...), which have 6 electrons in the d orbitals, are close to a Mott transition, but rather than the whole phase diagram as a function of doping is dominated by the distance from the Mott insulating global half-filling (5 electrons in the d orbitals) which plays the same role of the parent compound of the cuprates. I will review the experimental evidence for this and the theoretical understanding, based on an important role of the Hund's coupling leading to a strong differentiation between the orbitals [1]. This will lead to a surprising unification of the phase diagrams of cuprates and iron-based superconductors.

For the alkali-doped fullerenes I will discuss recent results combining ab-initio estimates of parameters with many-body methods which faithfully reproduce the experimental phase diagram of Cs<sub>3</sub>C<sub>60</sub> in which the ambient pressure Mott insulator turns into an s-wave superconductor under pressure, with a critical temperature which has a bell-shaped behavior which reminds the doping dependence in the cuprates [2]. This confirms previous theoretical studies suggesting that fullerenes are electron-phonon superconductors which benefit from strong correlations [3].

This work has been financed by FP7/ERC through the Starting Grant SUPERBAD (Grant Agreement 240524)

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**#314 - Vortex formation and dynamics in elongated Bose-Einstein condensates***Giacomo Lamporesi (I) - INO-CNR BEC Center*

*Other Authors: Matteo Barbiero, Franco Dalfovo, Michele Debortoli, Simone Donatello, Gabriele Ferrari, Fabrizio Larcher, Lev Pitaevskii, Simone Serafini, Marek Tylutki.*

I will report on the experimental observation of solitonic vortices in an elongated Bose-Einstein condensate.

A rapid quench across the BEC transition implies the spontaneous creation of defects in the phase of the resulting condensate [1], following the Kibble-Zurek mechanism. The most stable form of defects that lives long in the elongated BEC is represented by vortical lines, mainly oriented along the short axis of the BEC.

We study the properties of these stable topological defects (solitonic vortices) by imaging them from three orthogonal directions and through interferometric techniques [2, 3]. A stroboscopic method allows us to make a real-time imaging of a vortex orbiting in a BEC. We can detect the variation of the orbital period due to the atom number reduction on the long term, but also effects due to the interaction among vortices on the short term.

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**#315 - Solutions of the Two Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms***Luca Fausto Tocchio - SISSA*

*Other Authors: The Simons Collaboration on the Many-Electron Problem*

We present numerical results, obtained from a large collaboration, for ground state and excited state properties of the single-orbital Hubbard model on a two-dimensional square lattice, in order to provide an assessment of our ability to compute accurate results in the thermodynamic limit. Besides variational and diffusion Monte Carlo with a fixed node approximation, that will be described in more detail, many other methods are employed, including auxiliary field quantum Monte Carlo, bare and bold-line diagrammatic Monte Carlo, method of dual fermions, density matrix embedding theory, density matrix renormalization group, dynamical cluster approximation, unrestricted coupled cluster theory, and multi-reference projected Hartree-Fock. Comparison of results obtained by different methods allows for the identification of uncertainties and systematic errors. The importance of extrapolation to converged thermodynamic limit values is emphasized. Cases where agreement between different methods is

obtained establish benchmark results that may be useful in the validation of new approaches and the improvement of existing methods.

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1505.02290

### #316 - Localized Majorana-like modes in a number conserving setting

Davide Rossini - Scuola Normale Superiore

Other Authors: Fernando Iemini (1), Leonardo Mazza (2), Sebastian Diehl (3), Rosario Fazio (2) (1) Departamento de Física - ICEx - Universidade Federal de Minas Gerais, Belo Horizonte - MG, Brazil (2) NEST, Scuola Normale Superiore & Istituto Nanoscienze-CNR, I-56126 Pisa, Italy (3) Institute of Theoretical Physics, TU Dresden, D-01062 Dresden, Germany

We present an exactly solvable model of interacting fermions in a two-wire geometry [1]. Our model describes a topological superconductor supporting non-local zero-energy Majorana-like edge excitations and retains the fermionic number as a well-defined quantum number. The construction of the Hamiltonian with local two-body interactions and of its ground state draws inspiration from recent works on dissipative state preparation for ultracold atomic fermions [2], here applied to spinless fermions. The model has an exactly-solvable line, on varying the density of fermions, described by a topologically non-trivial ground state wave-function.

Moreover, by tuning the ratio of interaction vs. kinetic energy, we can further explore its properties outside the exactly-solvable line by means of the numerical density matrix renormalization group. We characterize its topological properties, establish the presence of a gap in its single particle spectrum while the Hamiltonian is gapless, and compute the correlations between the edge modes as well as the superfluid correlations. The topological phase covers a sizeable portion of the phase diagram, the solvable line being one of its boundaries. This finding is rationalized by pointing out a relation to the ferromagnetic XXZ chain.

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### #317 - Regularization of quantum fluctuations in the BCS-BEC crossover

Luca Salasnich - University of Padua

Other Authors: Flavio Toigo (University of Padua)

**I discuss very recent theoretical results [1,2] on the divergent zero-point energy of the superfluid Fermi gas in the BCS-BEC crossover.**

**The divergent zero-point energy**

**of the system is due to both fermionic single-particle excitations and bosonic collective excitations [1,2].**

**The regularization of the zero-point energy gives remarkable analytical results for composite bosons**

**in two dimensions [1] and in three dimensions [2].**

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### #318 - One-dimensional helium-4 beyond Luttinger theory

Mario Motta - Dipartimento di Fisica, Università degli Studi di Milano

Other Authors: Gianluca Bertaina (Dipartimento di Fisica, Università degli Studi di Milano), Maurizio Rossi (Dipartimento di Fisica e Astronomia, Università degli Studi di Padova), Ettore Vitali (Dipartimento di Fisica, Università degli Studi di Milano), Davide Emilio Galli (Dipartimento di Fisica, Università degli Studi di Milano)

We investigate zero temperature liquid  $^4\text{He}$  in strictly one dimension [1] by means of state-of-the-art Quantum Monte Carlo and analytic continuation techniques [2,3]. The system displays the unique feature of spanning all the possible values of the Tomonaga-Luttinger liquid parameter  $K_L$  by only changing the linear density. We explore the behavior of the dynamical structure factor beyond

the limits of applicability of Tomonaga-Luttinger liquid theory in the whole range of  $K_{\parallel}$ . We observe a crossover from a weakly interacting Bose gas regime at low density to a quasi-solid regime at high density, which we interpret in terms of novel analytical expressions for the spectrum of hard-rods [4]. During this transition the interplay between dimensionality and interaction makes the dynamical structure factor manifest a pseudo particle-hole continuum typical of a fermionic system, while the Bogoliubov mode evolves into a remnant of the roton mode. We provide also a perturbative estimation of the drag force experienced by a soft impurity moving along the system [5].

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### #319 - Meissner to vortex phase transition in hard-core bosonic ladders

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The phase diagram of a half-filled hard core bosonic ladder in a flux is investigated by means of Density Matrix Renormalization Group (DMRG) simulations and bosonization. We follow the transition from commensurate Meissner to incommensurate vortex state for increasing interchain hopping by calculating the leg current and the momentum distribution and we find that beyond a critical hopping the Meissner state is stable at any flux. For very high flux, we observe the formation of a second type of incommensuration in the vortex state that could be revealed in experiments with cold atoms. Other observables, like the rung current and bond-order wave correlations are also discussed.

### #320 - Vortex arrays in trapped Fermi gases throughout the BCS-BEC crossover

Pierbiagio Pieri - *University of Camerino*

*Other Authors: S. Simonucci and G. Calvanese Strinati*

Vortex arrays in type-II superconductors admit the translational symmetry of an infinite system.

There are cases, however, like ultra-cold trapped Fermi gases and the crust of neutron stars, where finite-size effects make it quite more complex to account for the geometrical arrangement of vortices. We self-consistently generate these arrays of vortices at zero and finite temperature through a microscopic description of the non-homogeneous superfluid based on a differential equation for the local order parameter, obtained by coarse graining the Bogoliubov-de Gennes (BdG) equations.

In this way, the strength of the inter-particle interaction is varied along the BCS-BEC crossover, from largely overlapping Cooper pairs in the BCS limit to dilute composite bosons in the BEC limit. Detailed comparison with two landmark experiments on ultra-cold Fermi gases, aimed at revealing the presence of the superfluid phase, brings out several features that makes them relevant for other systems in nature as well.

**#321 - Advances in the Time-resolved Imaging of Paintings**

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Time resolved luminescence imaging of paintings and pigments can yield maps of the distribution of different fluorescent and phosphorescent materials. In cultural heritage semiconductors are commonly found which exhibit long-lived fluorescence due to the presence of crystal defects and trapped ions. The instrumentation used for imaging which will be described in detail is based on coupling a ns laser (in our case the 2nd or 3rd Harmonic of a Nd:YAG emitting at 532 nm or 355 nm) to a time-gated intensifier. By varying the emission of the laser different luminophores are probed. Analysis of historical samples using time-resolved spectroscopy and complementary techniques allows a better understanding of the origin or luminescence in complex materials, many of which differ significantly from their modern equivalents. Examples of applications of luminescence imaging will include the detection and mapping of modern and ancient materials which include historical samples of lithopone and Egyptian blue, cadmium and other zinc-based pigments. Case studies and examples of analysis in situ will be shown to highlight the power of the technique to resolve details which complement multispectral imaging.

**#322 - Review on Digital Holographic Speckle Patterns Interferometry system and applications with emphasis on new results for environmental impact assessment in simulated climate conditions**

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In many artwork maintenance problems structural responses determine the conservation approach to sustain the long-term stability of the structure. The structural responses are primarily the dimensional changes caused by a physical or artificial impact forcing a change in the spatial coordinates. To measure changes of spatial coordinates an interferometric technique sensitive to optical path changes in three dimensions it is employed. The developed system based on the technique is termed Digital Holographic Speckle Pattern Interferometry (DHSPI) and is custom made to satisfy the critical boundary conditions required and be best suited in measurements for cultural heritage applications and especially the demand for portable system performance outside the laboratory. Examples of system application inside and outside laboratory are to be presented into a number of different conservation problems.

Also it is herein employed the optical laser geometry of holographic interferometry for providing the highest information content as it is the only method capable to capture dimensional effects rather than damage events only. The dimensional effects represent the impact of various factors onto the structure and the potential behavioral change of it whereas the damage events require fracture to take place. One of the most updated applications today favored of the holographic interference properties is the study of environmental effects on artwork structures and materials. In this paper the use of the DHSPI system in the study of the impact of environmental and climate or microclimate variability is presented. The relative displacement due to environmental changes is captured in remote real time automated operation allowing the continuous monitoring of surface displacement. The experimental methodology and procedure are presented with characteristic results.

**#323 - LUMINESCENCE DATING: RECENT RESULTS AND NEW PERSPECTIVES IN THE STUDY OF GLASS MOSAICS**

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The crystalline inclusions of ceramics (mainly quartz and feldspars) act as thermoluminescence (TL) dosimeters, the irradiation source being the natural radiation field. On this grounds various ceramic-like materials (pottery, bricks, cooked clays, bronze clay-cores) can be dated by TL. Similarly, Optically Stimulated Luminescence (OSL) has been exploited in more recent applications, using light instead of heat to detrapp electrons previously excited by ionising radiation.

In principle, Luminescence Dating can be used even with silica glass, once solved the main drawbacks of this application, i.e. the lack of crystallization and the transparency.

Up to now the feasibility of Luminescence Dating was investigated only with mosaic glass tesserae, a particular kind of glass, whose technology requires the addition to the basic mixture of different additive acting as coloring and opacifying agents. Many compounds were used through the centuries to make opaque glass, namely lead and calcium antimoniate and tin-based opacifiers. In some cases also grains of quartz were intentionally added to vitreous matrix with the same purpose.

Recent results [1, 2, 3] showed that the dosimetric properties of mosaic glasses depend on the presence of microcrystals in the silica network, sensitivity being possibly correlated to the crystallinity degree of the glass. Using specific techniques typical of the analysis of TL glow curves, like the "initial rise" following series of "partial cleanings" it has been possible to distinguish the TL emission due to the vitreous base of the tesserae from the emission given by crystalline micro-inclusions.

Various samples have been analysed through their TL and OSL emissions. Specific TL protocols have been developed to test sensitivity and sensitivity changes, the extent of optical bleaching and the signal regeneration by sunlight.

Despite the encouraging results, the protocols are far from being well defined, due to the difficulty in separating the vitreous component, strongly affected by anomalous fading, from the dosimetric component due to the crystalline micro-inclusions.

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#### #324 - Comparison between NMR and MIP in characterizing porosity of limestone used in Cultural Heritage

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Limestone with different porosity are used extensively as a sculptural and architectural stone in artistic-architectural field. As it is known, this kind of material is subjected to physico-chemical decay that involves the loss of surface and in-depth cohesion [1].

Consolidation interventions are performed in order to preserve building and decorative surfaces of architectural monuments, to reduce their degradation rate and to improve cohesion and adhesion in the stone [2].

Porosity of stone and pore size distribution are important factors to evaluate the effectiveness of a consolidation treatment and they are normally performed using a single technique such as mercury intrusion porosimetry, MIP [3]. Unfortunately, the instrumental limitations of this technique such as the assumptions on pore geometry lead to incomplete, sometimes deceptive results if used alone. Moreover, it leads to the destruction of the analyzed material and to the impossibility to test the same sample after a consolidation treatment.

Nuclear Magnetic Resonance (NMR) relaxometry of water <sup>1</sup>H nuclei can be also exploited to investigate pore space structure in high surface-to-volume ratio (S/V) systems (characterized by small pore size). NMR relaxation times of confined water depend on properties of the porous medium such as S/V and pore size distribution. Furthermore, in the last years portable devices for NMR relaxometry have been developed for *in situ*, non-destructive and non-invasive measurements consequently these instrumentations are able to analyze pore distribution before and after consolidation treatment [4].

In this experimental investigation results from NMR relaxometry and mercury intrusion porosimetry are compared with the aim at studying various type of limestone materials with different porosity. The performances of the two technique are compared and results are discussed. This analysis is preliminary for any investigation of the effectiveness of consolidation treatment.

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**#325 - Fano Physics on ultrashort time scales**

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Quantum states and resonances associated with transitions between them are among the most fundamental building blocks of physics and chemistry. To comprehensively understand states and resonances, it may be helpful to go beyond their (traditional) energy representation, and to study them from a time-domain perspective. This is particularly important for time-dependent interactions such as quantum systems exposed to weak or intense ultrashort laser fields, the key processes at the heart of time-resolved experiments.

The Fano mechanism describes a general physics phenomenon, traditionally understood as a resonance produced by an isolated state coupled to a continuum of states. This process plays a role across many scientific areas, including nuclear, atomic and molecular physics, optics, and solid-state physics. Applications are manifold, as the process builds a bridge between the microscopic (localized, bound quantum states) and the macroscopic world (continuum states, quasi-classical wavepackets) governing observables such as ionization yields or transport properties in matter.

Here, I will discuss time-domain measurements and laser control of atomic Fano resonances in helium atoms. Using extreme-ultraviolet (XUV) attosecond-pulsed light from high-harmonic generation (HHG), we study Fano resonances arising in the double-excitation of both helium electrons after the absorption of a single XUV photon. The XUV absorption spectrum was recorded after the passage of the broadband HHG pulse through a gaseous He medium, as a function of time delay and intensity of a synchronized and coherently locked near-visible (VIS) laser pulse.

The modification of the original Fano absorption profiles during the interaction with the VIS laser pulse can be understood by considering a single ultrafast time-domain phase control operation. As a result, the Fano resonance and the defining asymmetry ( $q$ ) parameter could be mapped onto a phase of the dipole response. This understanding also enables resonant amplification of light without inversion by a short-pulsed (impulsive) strong-field control operation, thus complementing the traditional dressed-state picture of electromagnetically-induced transparency. The same physical mechanism allows to measure quantum-state-resolved phase changes of individual doubly-excited states and thus to reconstruct a real-space representation of a laser-controlled two-electron wave packet. In the future, the ability to steer pairs of electrons that constitute molecular bonds may open new routes for laser-driven chemistry and reaction control.

**#326 - Attosecond photoemission time delay - another insight into electron correlation.**

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The understanding of ultrafast processes dynamics at the attosecond time scale ( $10^{-18}$  s) has revived interest in single photon ionization. Traditionally studied in the energy domain, photo-ionization was considered an instantaneous process. However recent time-resolved measurements of electron emission in atoms, molecules and solids shed light on a dispersion dynamic of the electron wave packets in a potential well [1-8]. Here we present work carried out in Lund aimed at characterising the influence of electron correlations on the attosecond dynamics of these wave packets.

The experiments were performed using attosecond pulse trains in the 30 to 42 eV photon energy range. Each pulse train corresponds to a frequency comb of odd order harmonics of an infrared laser (IR). The kinetic energy of the emitted electrons is analysed with a magnetic bottle spectrometer, which also allows for the coincident detection of particles (see Figure 1). The dispersion of electron wave packets in different noble gases is characterised by a technique of interferometry with an IR laser probe [9]. These measurements provide directly temporal information about the photoionization dynamics [8].

Supported by theoretical calculations, we show that the group delay of the electronic wave packet contains information about the nuclear potential after subtracting contributions related to the interaction with the probe laser [4, 5]. We show that it is possible to study the electronic correlations in the case of direct or resonant photoionization (Fano resonance) [6, 8]. Finally, we discuss the case of the double ionization of xenon where coincidence techniques allow us to identify the multiple double ionization mechanisms. [7] Hence, we can isolate the direct non-sequential double ionization mechanism and interpret our observations within a many-body perturbation theory in terms of shake-off and knockout mechanisms [10].

This methodology opens the door to the study of dynamics correlated multi-electronics and nuclear power in the molecules and aggregates.

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### #327 - Molecular orbital tomography by high-order harmonic generation

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High-order harmonic generation (HHG) driven by ultrashort laser pulses in matter represents a powerful tool for spectroscopy, providing insight into a number of properties of atomic and molecular species.

The imaging of the highest occupied molecular orbital (HOMO) by HHG in molecular gases [1] can be performed by measuring, in amplitude and phase, the harmonic field emitted by molecules for different molecular orientations with respect to the laser polarization direction.

Complex phenomena occurring during HHG, like multi-orbital contributions and the influence of the ionic Coulomb field, make the tomographic reconstruction procedure very difficult to apply to large molecules. A possible approach to overcome those issues is based on HHG by a few-cycle mid-infrared pulse [2] in an impulsively aligned molecular beam, where molecular alignment is induced by a second laser pulse.

In this work we report results obtained in some molecules (carbon dioxide,  $N_2O$ , acetylene); we show that, from the evolution of the harmonic spectra measured in those species as a function of the delay between the aligning and the driving laser pulses, it is possible to reconstruct the harmonic field emitted by the molecules both in amplitude and phase.

The reconstruction is based on a suitable retrieval algorithm, which takes into account the influence of the ion Coulomb field on the recolliding electron in a first order perturbative approach; the algorithm provides access to the emitted harmonic field as a function of the molecular orientation.

The map of the amplitude and phase of the harmonic field emitted by the target molecules can then be exploited for the reconstruction of their HOMO [3,4].

The mid-IR ultrashort laser pulses exploited in our experiments provide higher spectral cutoff energies and lower ionization levels with respect to standard Ti:Sapphire laser sources, thus enabling the HOMO reconstruction in fragile molecules with high spatial resolution.

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### #328 - Measuring photon correlations simultaneously in time and frequency

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Photon correlations are at the focus of research in quantum optics due to their ability to characterize the nature of a source from the relationship between emitted photons. With their seminal experiment, Hanbury Brown and Twiss provided the first evidence of inherent correlations between photons due to their bosonic nature. These correlations are described by the second order correlation function  $g(2)$ .

In this work we report a technical and conceptual advance by measuring simultaneously photon correlations both in time and frequency, by using a streak camera. This allows us to measure the full two-photon correlation spectrum (2PS) [1,2], a map of photon correlations in time-frequency space, for a condensate of exciton-polaritons. Unlike the usual approach using beam splitters and avalanche photodiodes, our procedure allows us to obtain both the energy and temporal information in only one measurement.

The resulting landscape of correlations shows an excellent agreement with the theoretical prediction, calculated thanks to a new theory of frequency-resolved correlations [3,4]. The 2PS unravels a richer dynamics of quantum emission than when disregarding the frequency as correlations are then washed out and reduced to a single number. We show how, on the contrary, the 2PS displays bunching in the diagonal ( $\omega_1 = \omega_2$ ) and color-antibunching in the antidiagonal ( $\omega_1 = -\omega_2$ ), providing the first observation of



anticorrelations at the single particle level in a condensate of exciton-polaritons. We show that the observed tendency of photons to clutter when they are equal and repel when they are different is not a specific feature of the system under consideration, but a general property of photon themselves due to its bosonic nature that can be described by a general bosonic form factor. This fundamental observation deepens our understanding of the nature of the intrinsic correlations between bosons, extending Glauber's conventional theory of photon correlations.

### #329 - Space-charge effects in hard X-ray photoelectron spectroscopy

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The development of the new X-ray free-electron lasers (FELs) opens new opportunities in the application of pump-and-probe techniques in photo-emission spectroscopy (PES) and offers new possibilities to investigate the ultrafast dynamics of the chemical, electronic and magnetic processes [1]. Moreover, excitation of the electrons by hard X-rays allows to overcome the strong surface sensitivity of conventional PES and to study the properties of buried (~nm) interfaces [2]. Despite these promising applications, the use of intense light pulses in PES is limited by the space charge created by the high number of electrons emitted at the same time, as evinced in experiments carried on with 3rd generation synchrotron radiation [3], ultraviolet lasers [4] and X-ray FELs [5]. Mutual interactions among the photoelectrons determine the broadening and the energy shift of the structures in the photoemission spectra. Theoretical models [6] and calculation procedures [7] have been implemented to predict the space-charge effects for future experiments. In this presentation we discuss the detrimental effects due to the space charge in the forthcoming PES experiments with hard X-ray (5-10 keV) pulses. Considering elemental metals as a case of study, we simulated the broadening of core-level peaks due to the interactions in the electron cloud using the Barnes-Hut many-body algorithm [8]. The numerous secondary electrons usually do not contribute to the typically observed photoemission structures but are the main responsible for the space-charge effects. The dependence of the energy broadening as a function of the number of photons per pulse and of the size of the beam spot on the sample surface is investigated. We found that the distortion of the energy distribution mostly occurs within few picoseconds after the emission and then in the very initial part of the flight of the photoelectrons and a time constant for the energy-broadening process can be easily estimated. The feasibility of pump-and probe photoemission experiments at new facilities like the European X-FEL with a tolerable energy broadening (0.1 eV or less) is discussed.

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### #330 - XUV-induced electron dynamics in aromatic amino acids

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Electron transfer within a single molecule is the fundamental step for many biological processes and chemical reactions. Theoretical studies have pointed out that very efficient charge dynamics can be driven by purely electronic effects, which can evolve on a temporal scale ranging from few femtoseconds down to tens of attoseconds

Here we report on a clear experimental measurement of charge migration in aromatic amino acids, after attosecond excitation. In our experiments, charge migration was measured by using a two-color, pump-probe technique. Charge dynamics was initiated by isolated sub-300-as pulses, with photon energies in the spectral range between 17 eV and 35 eV and probed by 4-fs, waveform-controlled near infrared (NIR) pulses, with central wavelength of 720 nm. A clean plume of neutral amino acids (phenylalanine and tryptophan) was generated by evaporation from a thin metallic foil heated by a CW diode laser. The ions produced by the interaction of the molecules with pump and probe pulses were then collected by a linear time-of-flight device for mass analysis.

In the case of phenylalanine we have measured the evolution of the yield of the doubly charged immonium ion ( $m/z = 60$ ) as a function of the delay between the attosecond pump pulse and the NIR probe pulse. By performing the measurement with a temporal resolution of 500 as we were able to identify the presence of a fast modulation of the dication yield with a periodicity of

4.3 fs. This fast dynamics can only be assigned to a pure electron dynamics, since nuclear dynamics usually comes into play on a longer temporal scale.

To better understand the observed dynamics, we performed numerical calculations. Despite the complexity of the charge dynamics triggered by the attosecond pulse, we were able to identify beatings between the amine and the carboxylic functional groups characterized by oscillation frequencies in good agreement with the experimental results. Electronic beatings were also identified in tryptophan, for which a modulation of the doubly charged immonium ion ( $m/z=79.5$ ) with a periodicity of 3.9 fs was measured. This ultrafast dynamics can be also associated to a charge migration. These ultrafast electronic processes constitute the first experimental measurements of charge migration in biologically relevant molecules.

### #331 - The hRIXS project at the European FEL

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An international user consortium will equip the SCS beam line of the European XFEL with a high resolution soft x-ray spectrometer for ultra-advanced resonant inelastic x-ray scattering (RIXS). The hRIXS project aims at adding the time resolution to high resolution RIXS studies, therefore hitting the intrinsic limit of Heisenberg uncertainty problem in x-ray energy loss spectroscopy. Moreover XFEL offers the opportunity to explore multi-photon processes, which could open the way to 4-wave scattering experiments in the x-ray regime.

The optical design of the 5 meter-long hRIXS spectrometer for the 300-1500 eV energy range, has been completed by the team of the Politecnico di Milano, in strict contact with the SCS beam line scientific staff, with the main partner and head of the Consortium (HZB), and with a number of other members of the Consortium.

The scientific goals, the technical and conceptual challenges behind hRIXS, and the final optical layout of the spectrometer will be presented.

The optical design work has been entirely covered by the PIK project "POLARIXS" of the MIUR (Italian Ministry of University and Research).

**#332 - A statistical benchmark for BosonSampling***Andreas Buchleitner (I) - Albert-Ludwigs-Universitaet*

Computing the state of a quantum mechanical many-body system composed of indistinguishable particles distributed over a multitude of modes is one of the paradigmatic test cases of computational complexity theory: Beyond well-understood quantum statistical effects, the coherent superposition of many-particle amplitudes rapidly overburdens classical computing devices - essentially by creating extremely complicated interference patterns, which also challenge experimental resolution. With the advent of controlled many-particle interference experiments, optical set-ups that can efficiently probe many-boson wave functions - baptised BosonSamplers - have therefore been proposed as efficient quantum simulators which outperform any classical computing device, and thereby challenge the extended Church-Turing thesis, one of the fundamental dogmas of computer science. However, as in all experimental quantum simulations of truly complex systems, there remains one crucial problem: How to certify that a given experimental measurement record is an unambiguous result of sampling bosons rather than fermions or distinguishable particles, or of uncontrolled noise? We describe a statistical signature of many-body quantum interference, which can be used as an experimental (and classically computable) benchmark for BosonSampling.

**#333 - Quantum information processing by quantum plasmonics***Stephane Guerin (I) - University Bourgogne Franche Comté**Other Authors: B. Rousseaux, D. Dzsojtan, G. Colas des francs, H.R. Jauslin (University Bourgogne Franche Comté)*

Controlling quantum emitters (atoms, molecules, quantum dots, etc.), light and its interactions is a key issue for implementing all-optical devices and information processing at the quantum level. This generally necessitates a strong coupling of emitters to photonic modes, as achieved by a high Q-cavity.

A nanoscale plasmonic platform has been envisioned to transpose strong coupling of quantum optics to plasmonics which takes advantage of the strong mode confinement of surface plasmon polaritons (SPP). Recent progress in quantum plasmonics showed the possibility of quantum emitters to reach the strong coupling regime to SPP fields. However, its application appears notoriously limited in practical situations due to the intrinsic presence of numerous and lossy modes, which complicates the description and the interpretation of the interaction, and introduces strong decoherence in the system. These drawbacks are known to limit severely the practical use of quantum plasmons for coherent manipulation of quantum emitters at the nanoscale.

In this presentation, we show how to solve these two issues. First, we derive an effective model from the fully quantized description allowing one to interpret the complete plasmonic coupling as a multimode lossy cQED interaction. The potential of our model is demonstrated in a second step: We show that we can engineer a specific coherent manipulation, where externally manipulating a pair of emitters coupled by SPPs, we make full use of the strong coupling while circumventing plasmonic losses via the use of unpopulated plasmonic modes. This is achieved by adapting the technique of stimulated Raman adiabatic passage (STIRAP), known to lead to an efficient and robust transfer of population between two metastable states commonly coupled to a lossy excited state, via a dark state immune to loss, thanks to adiabaticity usually reached for relatively modest durations and energies of the external control pulses. Here the STIRAP technique and its variant, the fractional STIRAP, are applied between the multi-emitter states driven by external fields: They allow the robust control of a complete or partial population transfer between two emitters, leading in particular to their high-fidelity entanglement.

**#334 - Nonequilibrium dissipation-driven steady many-body entanglement***Bruno Bellomo - Institut UTINAM - UMR CNRS 6213, Université de Franche-Comté**Other Authors: Mauro Antezza ( 1: Laboratoire Charles Coulomb (L2C), UMR 5221 CNRS-Université de Montpellier, Montpellier, F-France; 2: Institut Universitaire de France - 103, bd Saint-Michel, F-75005 Paris, France )*

This work concerns the manipulation of quantum systems by engineering the properties of the environment they interact with. It is based on recent studies regarding the properties of the radiation field produced in a given configuration when macroscopic bodies are kept at different temperatures [1]. Indeed, it has been shown that the interaction of small atomic systems (one or two atoms) with a field produced in a configuration kept out of thermal equilibrium may permit a strong manipulation of the atomic dynamics [2-5].

Here we study an ensemble of more than two two-level quantum systems (qubits) interacting with a common electromagnetic field in proximity of a dielectric slab whose temperature is held different from that of some far surrounding walls.

We show that the dissipative dynamics of the qubits driven by this stationary and out of thermal equilibrium field, allows the production of steady many-body entangled states, differently from the case at thermal equilibrium where steady states are always non-entangled. By studying up to ten qubits, we point out the role of symmetry in the entanglement production, which is exalted in

the case of permutationally invariant configurations. In the case of three qubits, we find a strong dependence of tripartite entanglement on the spatial disposition of the qubits, and in the case of six qubits, we find several highly entangled bipartitions where entanglement can, remarkably, survive for large qubit-qubit distances up to 100 micron [6].

Our analysis points out the potentialities of rich yet simple configurations involving macroscopic bodies held at different temperature, which are within experimental reach. They may permit the production and manipulation of steady multipartite entanglement, resistant for large inter-qubits distances, offering then new tools possibly exploitable for quantum computational tasks. All this is obtained without any further external actions on the qubits, being the result of the qubits dissipative dynamics itself. These protocols are then intrinsically robust to environmental effects and do not need of initializing the total system in a given configuration.

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### #335 - Thermally activated nonlocal amplification in quantum energy transport

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We study energy transport efficiency in 2D and 3D configurations of two-level atoms. We show that, if these systems are embedded in a common blackbody radiation, the transport efficiency can be greatly increased with respect to the case at  $T=0$ . To understand this phenomenon we exploit the exact knowledge of field self-correlations, and show that excitations can travel along the atomic system due to two alternative physical effects: in addition to the standard excitation hopping thanks to the atomic dipole interactions, atoms can affect each other's internal energy also by collective dissipation induced by non-local self-correlations of the electromagnetic field. This latter term has been neglected in previous phenomenological approaches since its effect has been assumed to be negligible. Although this assumption is well justified for regular systems where hopping dominates, it breaks down in more general, non-regular configurations. By a microscopic analysis of atomic dynamics, we show that these non-local terms, triggered by the thermal noise induced by the blackbody radiation, play a fundamental role in atomic energy transport. This generates a counter-intuitive temperature dependence of transport efficiency, which gets largely amplified in certain ranges of temperature. Thanks to this effect excitations can travel along paths where hopping is forbidden, with efficiencies remarkably higher than 100%

### #336 - Spanning the full Poincaré sphere with polariton Rabi oscillations

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The coupled dynamics of exciton and photon in semiconductor microcavities produces light-matter oscillations (polariton Rabi oscillations) ruled by the time-dependent occupation of the eigenstates of the system (upper and lower polariton branches). Here, thanks to a comprehensive model of exciton-polariton Rabi dynamics and a digital holography technique for ultrafast spectroscopy of the polariton emission, we show how the time-dependent intensity and polarization of the emitted light can be precisely controlled by consecutive pulsed excitation of the system. Experimentally, the intensity of the emission is given by the photonic part of the polariton field, while the complete evolution of the system is described by a fundamental model of coupled bosonic fields. Interestingly, also the Poincaré sphere in the polarization basis can be spanned in time intervals as short as 10 ps, with a full control of the polarization dynamics on a femtosecond timescale.

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### #337 - Matter-Wave Interferometry of a Levitated Nanodiamond Induced and Probed by a Spin

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Quantum mechanics has always puzzled scientists because its features do not seem to be valid in everyday life, as exemplified by the well known paradox of Schroedinger's cat, where a cat can be in a superposition of dead and alive states. Since quantum mechanics works extremely well when we describe the microscopic world, there must be a boundary which establishes to what extent the theory gives the correct predictions and when the microscopic world becomes macroscopic.

Optomechanics is a new field of quantum optics whose aim is to test the validity of quantum mechanics with objects (such as vibrating mirrors interacting with the quantized electromagnetic field) which we would like to take bigger and bigger.

In our contribution, we propose a novel optomechanical system, where an oscillating nanodiamond interacts with the spin of a defect embedded in it. The spin-motion coupling is realized by means of a suitable magnetic field gradient, which induces a spin-dependent conditional displacement on the center of mass of the bead. We show that the evolution of the spin evidences phases which come from the interaction of the diamond with the gravitational field. The possibility of revealing quantum superpositions of the motional states of the nanodiamond by measuring the spin only may considerably simplify future tests of the validity of quantum mechanics and shed new light on our understanding of the microscopic/macroscopic transition. To this aim, we consider also extensions of our scheme which would allow us to test models of quantum collapse with our device.

Finally we discuss practical metrological applications aimed at building miniaturized gravimeters.

### #338 - Direct evidence of Rabi oscillations and anti-resonance in a strongly coupled organic microcavity

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Cavity polaritons exhibit a wealth of fascinating phenomena, due to the strong coherent coupling between their photonic and excitonic components. The microscopic origin of these phenomena lies in the coherent interaction between excitons and cavity photons, via coupling of the excitonic transition dipole moment to fluctuating (vacuum) electromagnetic fields stored within the cavity. This strong coupling results in the formation of new hybrid lower (LP) and upper (UP) exciton-photon polariton modes, separated in energy by the normal mode splitting.

In our work, we report the direct observation of 30-fs period Rabi oscillations between excitons and cavity photons in a strongly coupled J-aggregate microcavity<sup>[1]</sup>. The transmission of ultrashort pulses through the polariton modes was temporally resolved using time-resolved up-conversion to reveal ultrafast coherent exchange of energy taking place at a Rabi time period of about 30fs for a Rabi splitting energy of about 140meV at room temperature. Further evidence of strong coupling in the microcavity was obtained using linear spectral interferometry. The phase of transmitted electric field through the angle-tuned microcavity was extracted. Distinctive anti-resonance feature, typical of coupled systems, was observed at the resonant absorption frequency of the J-aggregate exciton. This antiresonance selectively probes the uncoupled exciton excitation, and its observation uncovers the coherent and ultrafast exchange of energy between the optically excited cavity and the J-aggregate excitons. As expected for the exciton absorption mode, this anti-resonant phase shift was dispersion-less with respect to angle-tuning. The time domain Rabi oscillations as well as the frequency domain anti-resonance feature were well supported by theoretical simulations of the strongly coupled microcavity.

[1] S. K. Rajendran et al, *Direct evidence of Rabi oscillations and anti-resonance in a strongly coupled organic microcavity*. Physical Review B 91, 201305(R) 2015.

### #339 - Ultracold atomic bosons in double, triple, and four-well potentials.

Giovanni Mazzaella - Università degli Studi di Padova-Dipartimento di Fisica e Astronomia "G. Galilei"

We consider ultracold atomic bosons confined in double, triple, and four-well shaped potentials. We study such systems within the framework of the (two,three,four-site) Bose-Hubbard model. By varying the atom-atom interaction, we investigate the bosonic ground state. This latter exhibits a variety of forms ranging from the coherent state in the delocalization regime to a macroscopic cat-like (in the case of two and three spatial modes) and two-pulse states (four-site configuration) with (quasi)-fully localized populations.

### #340 - Critical behaviour of ultra-cold bosonic gases in a confining potential

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Experiments with ultra-cold atoms use a confining potential to keep the sample trapped in place. However, the presence of the trap is most often neglected in the modelling and analyses, in favour of treatments based on homogeneous descriptions. The trap qualitatively modifies the critical behaviour of these systems near a phase transition: most notably, it bounds the correlation length to remain finite.

The trap-size scaling can provide a sound treatment of the effects of the confining potential. In this seminar, I shall review some general aspects of trap-size scaling. I shall then concentrate on its application to the three-dimensional Bose-Hubbard model, which realistically describes a bosonic gas in an optical lattice.

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**#341 - Tracking fast electrons at organic interfaces by core hole clock spectroscopy**

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Understanding the interplay between molecular bonding and charge transfer pathways in heterojunctions is a key issue for molecular engineering and design of novel organic nanodevices. Experimentally, different pathways for carrier transfer within molecular assemblies can be probed with resonant photoemission (RPES) by measuring the time of electron and/or hole delocalization from the specific site of creation. The detection of ultrafast charge delocalization may then reveal the preferred pathways for carrier transport and provide unique insight in the origin of the nanoassembly's conductive properties. The basics of core-hole-clock (CHC) experiments [1] of the RPES will be presented in relation to various organic molecular systems. Ultrafast electron dynamics in amine terminated and pyridine based molecular overlayers on Au(111) will be presented in relation to recent results of single molecule break junction experiments that may provide a direct comparison between quantum and mesoscopic properties of such systems. The models used to extract the time scale of the excited charge delocalization and the spatial correlation of core and valence molecular states will be briefly discussed. CHC measurements of fast electron dynamics in a few organic systems with p-pand donor-acceptor molecular coupling will be presented to evidence the essential coupling motifs for efficient transport in molecular junctions [2].

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**#342 - Energy level alignment at metal-organic interfaces probed via molecular self-assembly**

Giovanni Costantini (I) - University of Warwick

Most applications in organic electronics and organic photovoltaics require the deposition of a thin molecular film onto conductive electrodes. The growth of the first few molecular layers represents a crucial step in the device fabrication since the organic-electrode interface carries the entire device functionality. Nevertheless, the ability to rationally tune and modify the electronic configuration of these systems is extremely limited because the energy level alignment at metal-organic interfaces is influenced by a complex combination of factors. As a result, most work in the field is still based on a trial-and-error approach.

In this talk I will present a new method to investigate the formation of metal-organic interfaces based on studying the relation between molecule-substrate charge transfer and the development of specific molecular assembly patterns. In particular, I will show that the driving force for charging an individual molecule depends not only on the position of its frontier orbitals with respect to the substrate Fermi level, but also on the electrostatic interaction with its local neighbours' environment. The resulting interplay of long-range attractive or repulsive forces acting between interfacial molecular dipoles and short-range attractive interactions, determines the emergence of peculiar assembly patterns that are a direct consequence of the local electronic configuration.

Using a series of ad-hoc designed molecules I will show that combining scanning tunnelling microscopy and spectroscopy with atomistic simulations allows to study the elementary processes responsible for the observed self-assembly behaviour. The talk will focus on molecules characterised by anomalous coarsening caused by reversible charge transfer [1] and on two-component systems where specific co-assembly patterns result from the electron accepting behaviour of one molecule being selectively induced by the presence of the other [2].

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**#343 - Cu Chiral Nanostripes induced by Metal Organic Complexes**

Celia Rogero (I) - Centro de Física de Materiales (CSIC/UPV/EHU)

The trend of miniaturization to the nanoscale that new technological devices are promoting requires a detailed control of the processes that take place at this level, and represents a significant challenge in every aspect of the design and manufacture. In particular, fields such as surface engineering, electrochemistry, catalysis or energy demand the use of specific and carefully controlled physical-chemical processes at nanostructured surfaces. This opens the way to study, for example, on-surface reactions, crystal growth, or chirality of photoactive molecules on surfaces for applications in solar cells, pharmacology or spintronic.

In this context, our work is focused on the study of tetrapyrrole molecules, phthalocyanines, on Cu(110). Combining multiple surface science techniques—Scanning Tunneling Microscopy (STM), X-ray Photoelectron Spectroscopy (XPS), or Near Edge X-ray Absorption Spectroscopy (NEXAFS)—with Density Functional Theory (DFT) we have investigated a novel molecular/substrate interaction mechanism [1]. We determine that varying the nature of the central macrocycle, from non-metalated to metalated

molecules, it is possible to control the adsorption of the molecules from being just physisorbed to inducing a complete reshaping of the surface. This derives in the formation of chiral arrays of Cu nanoribbons even when the molecules are achiral. At variance with the conventional changes of metal reconstructions upon molecular adsorption observed so far, the presented faceting is found to involve a massive reorganization of Cu adatoms. The energy gain of the final system comes not only from the preferential adsorption position of phthalocyanines on the copper surface, but also from their interaction with the surrounding adatoms. We demonstrate that indeed the mechanism behind the massive surface reshaping involves a molecular mediated uni-directional blocking of diffusing surface adatoms.

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#### #344 - Unoccupied surface features induced by epitaxial graphene on metal surfaces

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##### Unoccupied surface features induced by epitaxial graphene on metal surfaces

The interaction between graphene and metal surfaces has been often classified as strong or weak depending on the degree of destruction of the Dirac cone, as due to the hybridization of graphene states with the d band of the metal. Nevertheless away from the Fermi level, in the unoccupied spectrum, graphene always shows relevant perturbing effects on the surface states localized outside the surface. Although these states are a very sensitive probe for understanding the graphene-substrate coupling and can significantly affect the electron dynamics at the surface they are poorly characterized, especially from an experimental point of view.

We present a joint experimental-theoretical work exploiting angle-resolved nonlinear photoemission technique and Density Functional Theory calculations to characterize the unoccupied spectra of graphene on different metal surfaces, namely Cu(111), Ni(111), Ir(111).

We show that both in strongly (G/Ni) and weakly (G/Cu) interacting systems the variations of electronic potential in the vacuum region give rise to the appearance of a quantum well state localized between the surface and graphene layer.

Furthermore the carbon layer affects the screening charge of the surface leading to partially modified image states with respect to the clean surface.

We characterize these features in term of their binding energy, effective mass, spin character and wave function. We found that the energetic and spatial proximity of the quantum well state and the first image state can give rise to hybridization effects, as in the case of G/Cu.

The epitaxial graphene determines also a decrease of the metal surface work function. On Ir(111) this allows to efficiently populate, by using photon energies in the near ultra-violet region, the first image state at  $k_{\parallel} \neq 0$  different from the Gamma point. For the first time, we report on the experimental evidence of a Rashba-type spin splitting in  $n = 1$  image

potential state, that we find to be five times smaller than one measured on the same surface on

the occupied SS. On the basis of theoretical considerations we show that this difference can be ascribed both to the smaller amplitude and asymmetry of the image state charge density with respect to the SS around the Ir nuclear position.

#### #345 - Simulating Scanning Tunneling Spectroscopy through quantum Monte Carlo

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Scanning tunnelling spectroscopy (STS) is an experimental technique able to visualize electronic states in nano-objects, such as quantum dots or molecules. Ideally, through Scanning Tunneling Spectroscopy (STS), the many-body observable that is accessible at low temperatures is the spectral density resolved in space and frequency.<sup>1</sup> After integrating over the energy in a neighborhood of the electrochemical potential, one obtains a positively defined function that can be regarded as the square modulus of the quasi-particle Wave Function (QPWF) (or Dyson orbital) of the electron that is subtracted (hole QPWF,  $hQPWF$ ) or added (electron QPWF,  $eQPWF$ ) to the  $N$  electron molecule during the STS experiment.<sup>2,3</sup>

Therefore, the spectra and topological images of STS sometimes contain fundamental contributions from electronic correlation and have thus been proposed as a way to visualize these correlation effects in quantum dots and molecules.<sup>1-3</sup> A computational method able to go beyond the single particle representation is needed to highlight such effects, and recently, to this end, different



approaches have been devised using ab initio methods like Configuration Interaction (CI) and Coupled Cluster (CC), both truncated at the second order expansion (CISD, CCSD).<sup>3</sup>

In this work we present a quantum Monte Carlo (QMC) algorithm to calculate the  $h$ QPWF and the  $e$ QPWF with a procedure that extends the correlated sampling technique<sup>4</sup> already used to calculate energy differences and wave function overlaps in QMC. With this procedure we overcome different limitations of the previous ab-initio approaches, recovering an higher level of electronic correlation.

In particular, we present first results on molecules at the Variational Monte Carlo (VMC) level, using the Jastrow Antisymmetric Geminal Power (JAGP) wave function<sup>5</sup> which is able to recover both the dynamical and the static contributions to the electronic correlation of various molecular systems such as diradicals.

This work is supported by MIUR- PRIN 2012 MEMO.

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### #346 - Two-dimensional metal-organic network synthesis and characterization

Matteo Lo Cicero - Department of Chemistry, University of Rome, "La Sapienza"

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The development of synthetic routes leading to ordered and periodically well-defined two-dimensional (2D) covalent molecular sheets, would open-up unique technological and theoretical aspects, which are likely to present a huge impact on the nanoscience and nanotechnology using advanced materials [1].

Metal-organic polymeric networks constitute particular intriguing and interesting self-assembled 2D systems, formed by metal atoms and organic ligands. If the metal is magnetic, this kind of systems can provide a groundwork for high-density memory devices with low energy magnetic switching, due to the presence of an easy magnetization axis, and high operation rate. Such systems may be also designed to mimic the catalytic centers of some types of enzymes for potential biological applications [2].

The network we present in this work is based on tetrahydroxyquinone (THQ) molecules deposited on single-crystal Cu(111). Molecular monomers temperature dependence surface-assisted dehydrogenation and resulting surface metal adatom extraction evidences will be shown. Due to overlayer adatom extraction and small-size monomers, this particular system present peculiar sub-nanometric intermetallic distances, feature that makes it particularly interesting within spintronic field.

THQ/Cu(111) system thermal activation, lead to covalent metal organic network synthesis. We report detailed experimental X-ray photoelectron spectroscopy (XPS) measurements concerning observed surface-assisted THQ dehydrogenation, as a function of time and temperature. Chemical bonds breaking and formation has been followed by core level energy measurements. Several 2D ordered phases formed at different temperatures, have been characterized by low-energy electron-diffraction (LEED). Finally, preliminary scanning tunneling microscopy (STM) measurements at nanometric scale, confirmed geometries provided by LEED. Information like unitary cell size and azimuthal orientation of both monomeric and polymeric adsorbate are presented.

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### #347 - PDIF-CN2 organic thin-film deposited at room temperature by supersonic molecular beam deposition for n-type OTFT

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The possibility to get high-mobility n-type transistors avoiding thermal treatments during or after the deposition could significantly extend the number of substrates suitable to the fabrication of flexible high-performance complementary circuits. In this contribution, we report on the fabrication of N,N'-1H,1H-perfluorobutildicyanoperylenediimide (PDIF-CN2) organic thin-film transistors (OTFT) by Supersonic Molecular Beam Deposition (SuMBD) on silicon dioxide dielectric treated with

Hexamethyldisiloxane (HMDS) in the bottom contact-bottom gate configuration. The best device exhibited mobility ( $\mu$ ) up to 0.2 cm<sup>2</sup>/Vs even if the substrate was kept at room temperature during the organic film growth. This  $\mu$  value exceeds by three orders of magnitude the electrical performance of PDIF-CN2 films grown at the same substrate temperature by conventional Organic Molecular Beam Deposition (OMBD). This achievement is possible thanks to the high kinetic energy ( $E_k$  is at most 18 eV) reached by the molecules during SuMBD process, where  $E_k$  plays very effectively the equivalent role of the substrate temperature in the OMBD technique [1]. By SuMBD, however, the PDIF-CN2 film growth turns out to be very critical with respect to the deposition parameters (in particular the deposition rate). For example, it is possible to observe the critical dependence of the measured charge carrier mobility on the deposition rate assumed during the film growth. Moreover, it was observed that the reported final electrical response can be obtained only waiting for some days after the deposition. Just after deposition, indeed, these OTFT display very poor electrical performances. This effect is associated to a post deposition crystallization and molecular reorganization effect monitored through Atomic Force Microscopy and X-ray diffraction measurements.

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**#348 - Graphene Based Gas Sensors**

Wojtek Wlodarski (I) - RMIT University

GRAPHENE BASED GAS SENSORS Wojtek Wlodarski School of Electrical and Computer Engineering RMIT University Melbourne, AUSTRALIA The application of graphene for the gas sensing has become recently a new fast growing area of interest. Graphene has the tremendous potential for development of gas and vapour sensors. This is in part due to the fact that each atom in the structure interacts directly with the sensing environment and in part due to the ease with the electron properties of graphene can be modified by this interaction. Graphene and related materials could be combined with different transducing platforms such as: conductometric, Surface Acoustic Waves (SAW), Bulk Waves (BW), Schottky diodes, mass sensitive, Field Effect Transistors (FET), optical as well as based on the noise spectra measurements. Combining these transducers with graphene results in the development of new generation of sensitive, reversible and stable gas and vapour sensors with several advantages which will be discussed. Numerous examples of recently developed gas and vapour sensors for NO<sub>2</sub>, CO, CO<sub>2</sub>, SO<sub>2</sub>, H<sub>2</sub>, NH<sub>3</sub>, CH<sub>4</sub>, VC and H<sub>2</sub> will be presented.

**#349 - Trace gas detection through a comb-locked cavity-ring-down spectrometer**

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High-sensitivity detection of gases is obtained with a novel comb-locked cavity-ring-down spectrometer operating in the near-infrared, from 1.5 to 1.63 micron. Key feature of the approach is the tight frequency locking of the probe laser to the comb, ensuring very high reproducibility and accuracy to the frequency axis upon scanning the comb repetition rate, as well as an efficient light injection into a length-swept high-finesse passive cavity containing the gas sample. Spectroscopic tests on carbon dioxide demonstrate a limit of detection as low as 5.7·10<sup>-11</sup> cm<sup>-1</sup> together with an accuracy of ~36 kHz on the determination of the line centre frequency in a Doppler broadening regime over the time scale of about 5 minutes, corresponding to four consecutive spectral scans of the absorption line.

**#350 - Different techniques, compared for the indigenous mould characterisation**

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Mould contamination of food and feed it's a worldwide concerning problem due to the production of harmful metabolites like micotoxins by this microorganisms.

The early detection of the occurrence of these contaminants became mandatory to assure food safety and to avoid economic losses in industry.

Current detection methods require time, special skills, and are still quite expensive.

The aim of this study was to compare and find the fast, economic technique for the early detection and identification of mould contaminants in different foodstuff.

The preliminary part of this work was performed isolating mould from food matrix. To isolate and select, 4 different kinds of *Aspergillus Niger*, 2 kinds of *Aspergillus Flavus*, 1 *Aspergillus Ochraceus*.

Classical microbiological, chemical and optical techniques were compared in this work. GC-MS with an autosampler SPME and a Small sensor system (S3) device equipped with an array of 6 chemical metal oxide nanowire gas sensors has been selected [1].

Nanowire sensor arrays has been prove to be a remarkable tool to be use in food quality control and safety [2][3].

Fundamental cooperation to obtain the creation of "Standard Mold Map" (SMM). SMM will be able to distinguish unequivocally the mould species.

The subsequently part was used to identify the faster/cheaper and useful method to create the SMM. In particular, several molds were characterized by spectroscopic methods, Vis/UV absorption, fluorescence and FTIR absorption [4].

The varieties of techniques used in this work strongly suggest the use of SMM techniques able to distinguish univocally the mould species.

**Acknowledgment**

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### #351 - MULTI-FUNCTIONALIZATION OF GRAPHENE OXIDE FOR SENSING APPLICATIONS

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The present work tackles the functionalization of graphene oxide (GO) sheets to fabricate multifunctional nanoplatfoms whose assembly states can be controlled in response to different stimuli for *in-vitro* diagnostic application. Specifically, a versatile and smart GO-based substrate - responsive to pH (chemical stimulus), temperature (physical stimulus) and enzymes (biological stimulus) - was prepared by covalent and/or non-covalent binding respectively of acrylates, acrylamides and dye-labeled peptides onto the GO surfaces. The latter GO functionalization was achieved both by simple physisorption, through hydrophobic and pi-pi interactions, and by the grafting of reactive amino-groups via nitrogen-argon plasma treatment. The microwave plasma was created by a surfaguide pulsed at 2.44 GHz, and the plasma discharge was set in pulsed mode. To avoid an overheating and a massive etching of the carbonious matrix of the GO, the sample was collocated in the post discharge zone of the plasma, where a flux of H<sub>2</sub> was introduced during the plasma treatment, to increase the amino selectivity. This configuration was found the most efficient to achieve a good grafting yield and selectivity, keeping at the same time the integrity of the surface.

The cooperative effects due to the manifold functionalization were scrutinized with a multitechnique approach of spectroscopic (Raman, X-ray photoelectron spectroscopy, UV-visible, fluorescence) and microscopic (confocal and atomic force microscopy, scanning electron microscopy) methods, both in solution and at the solid surface. In addition, *First Principle* and *Molecular Dynamics* calculations were performed in parallel with the experiments. Results indicate the promising performances of the developed nanomaterials for the understanding control of the processes, both kinetics and thermodynamics aspects, at the graphene-(bio)molecule interface as well as for the (bio)molecule-target interaction in solution.

### #352 - Metal Oxide Nanowires preparation and integration in chemical sensing devices

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Oxides materials show properties covering almost all aspects of material science and physics in areas including oxide electronics, superconductivity, ferroelectricity, magnetism...

Metal oxide nanostructures are studied in many areas such as solar cells, TFTs, LEDs, energy harvesting for their functional properties. In the field of health and wealth they can be used as gas sensors to detect toxic gaseous species or to monitor chemical compounds that may be related to the well being of a person. Acetone for example is useful for diabetes monitoring. In fact, the people suffering from diabetes have a particular breath odor, because of producing large amount of acetone through their normal metabolic processes.

Metal oxides are already established in the field of gas sensing, the sensing mechanism consists in an electrical resistance variation upon gas chemisorption. The advantages of using single crystal nanowire of metal oxides compare to films are: a very large surface-to-volume ratio, the downsizing of sensing materials that improves the sensor performances, their stability (high degree of crystalline order), the higher capability to accommodate strain in presence of lattice mismatch, while the main challenges remains the integration in macroscopic devices with good and stable electrical contacts.

Oxides like tin, zinc, copper, nickel, tungsten and niobium oxide were synthesized by vapor-liquid-solid technique, thermal oxidation or hydrothermal methods. Functional properties of these structures as gas sensors were tested to different pollutants and towards acetone at different working temperatures, showing the capability to use the devices in real applications.

**#353 - Multipurpose lab on chip – From medical diagnostics to food and environmental monitoring**

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Recently the development of lab-on-chip devices attracted large interest for detection of specific analytes/markers, cellular studies, drug screening as well as food and environmental monitoring. In this respect, electrochemical impedance spectroscopy is a powerful tool.

Here the development of a multipurpose biochip with integrated microfluidic components is described. Specifically, the layout consists of various sensing areas, each one including an array of transducers (gold interdigitated electrodes), while microfluidic channels are used for the delivery of functionalization and sample solutions into the chambers. Such biochips are first demonstrated to be suitable for viability assays, cytotoxicity tests and migration assays on cell populations<sup>1</sup>. Then other applications are discussed concerning the ultrasensitive (pM) detection of biorecognition events in flow immunoassays, such as in the case of cholera toxin in solution or cancer biomarkers in sierra<sup>2</sup>.

Our recent publications demonstrate that these biochips are very suitable for clinical analysis, being faster and more reproducible than traditional techniques. In particular our attention was so far focused mainly on cancer diseases. For example, by means of appositely developed biochips, we assessed the presence of autoantibodies against Ser-419-phosphorylated ENOA in sera originating from patients with pancreatic ductal adenocarcinoma (PDAC)<sup>3</sup>. Biochip results are in agreement with those from traditional techniques, such as ELISA and Western Blot, but measurements are much more sensitive and specific increasing the possibility of PDAC diagnosis. Similar chips also allowed to evaluate the free-to-total PSA ratio useful for screening of prostate cancer risk<sup>4</sup>. On a different approach, these biochips were modified to enable automatic tests to quantify the invasive potential of cell lines by detecting the migratory activity of hepatocellular carcinoma (HCC) cells as a function of microenvironment<sup>5</sup>.

Similar biochips were also applied for food and environmental monitoring. For example, we recently reported a portable gliadin-immunochip for contamination control on the food production chain which was validated for both liquid and solid food matrixes by analysing different beers and flours<sup>6</sup>.

Presently, we are integrating monolithic valves for fluid handling using thermo-responsive hydrogels<sup>7</sup>.

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**#354 - Integration of magnetic tunneling junction based devices in a portable platform for biosensing applications**

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In recent years, magnetoresistive (MR) biosensor arrays combined with magnetic markers have emerged as a new promising platform for biosensing. The most widely used scheme relies on the detection of molecular recognition events between the probe molecules, bound onto the sensor surface, and the magnetically labeled target molecules, which bind specifically to the complementary probes. The magnetic field of the superparamagnetic labels on the surface of the sensor causes a change in the electrical resistance of the sensor, which is related to the concentration of the immobilized target molecules. In this work, we demonstrate the detection of natural DNA hybridization events from different classes of pathogens, precisely Hepatitis E virus (HEV) and Pathogenic bacteria (*Listeria monocytogenes*), using highly sensitive magnetic tunneling junction (MTJ) based devices. The sensor stack is deposited by magnetron sputtering and processed by optical lithography and ion milling [1][2]. Moreover, we successfully integrate the MR devices in a portable, compact platform provided with in-built electrical and fluidic apparatus. Our results show that the platform successfully meets the requirements for the detection of hybridized natural DNA. Moreover, this work represents a fundamental step towards the integration of MTJ-based biosensing platforms in compact Lab-on-a-chip devices for the straightforward detection of pathogens in the agrifood industry and for further medical applications. [1] Albisetti E. et al. *Biosensors & Bioelectronics* 47, 213–7 (2013). [2] Albisetti E. et al. *Sensors and Actuators B* 200 (2014).

**#355 - Recent developments in photoluminescence-based chemical sensing by nanostructured metal oxide materials**

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Metal oxide (MOX) nanoparticles are at the basis of many important applications including chemical sensing (e.g. tin and zinc oxide), heterogeneous photocatalysis and environmental remediation (e.g. titanium dioxide) and solar energy conversion (e.g. zinc oxide, titanium dioxide). These properties are decisively controlled by MOX photophysical characteristics.

Ambient-controlled Photoluminescence (PL) analysis provides important information on these latter characteristics, while also representing a possible multi-parametric route to chemical sensing. Our recent researches in this field focused on (A): fundamental studies on interactions between polluting gas molecules (e.g. ozone, NO<sub>x</sub>, volatile organic compounds et al) with MOX nanoparticles and on (B): application of MOXs as optical nanosensors. These topics are investigated through different variants of PL technique (static, excitation-resolved, time-resolved).

In this contribution we debate on some recent findings shading light on the possible "static quenching" mechanism that drives the response of ultraviolet emission in zinc oxide ZnO toward oxidizing molecules. Moreover, we discuss on the feasibility of the use of *mixed-phase* TiO<sub>2</sub> for efficient and multi-parametric oxygen sensing. In this latter case, we evidence that O<sub>2</sub> produces opposite responses in rutile and anatase photoluminescence efficiency, highlighting interesting potentialities for future double-parametric optical sensing based on titania.

The results underline an important role of lattice oxygen atoms, suggesting that the standard Schottky barrier mechanism driving the response toward gas species in most used metal-oxide sensors (e.g., tin dioxide) is not the only active mechanism in TiO<sub>2</sub>. This is of great importance in understanding and explaining the known differences existing between TiO<sub>2</sub>-based gas sensors and those based on a standard chemoresistive material, namely SnO<sub>2</sub>.

A physical model explaining the different effects induced by oxygen on the PL activity of the two TiO<sub>2</sub> polymorphs will be presented, also underlining how such a proposed mechanism can drive PL-based optochemical toward improved performances of interest for applications.

### #356 - Integrated wearable sensors for elderly people critical event detection in home environment

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This paper presents a multi-sensor wearable system for the detection of people critical events in the home environment. The main reason for the development of the presented integrated and wearable multi-sensor-system is to allow non completely self-sufficient people (e.g. older people) to live comfortably in their own houses as long as possible and since one of the major causes of injury and fear for older people is the risk of critical and dangerous events, technology should be exploited to automatically provide fast assistance when needed. In particular, the developed sensor system, in case of emergency, communicates with care holders and relatives of the assisted person through an internet-based gateway. Furthermore, in order to prevent false alarms the use of redundant or multi-sensory systems is mandatory. Details on materials and technologies for sensors and MEMS fabrication on flexible substrate will be also provided.

### #357 - AlN texturing and piezoelectricity on flexible substrates for sensor applications

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We show that AlN-based piezocapacitors with relatively high piezoelectric coefficient ( $d_{33}$ ) values (3-4 pC/N) can be fabricated on polyimide (PI) substrates at 160 °C or even at room temperature by sputtering processes. With respect to PI, a reduction of the piezoelectric performances was observed on polyethylene naphthalate (PEN). With the same approach, a  $d_{33}$  value as high as 8 pC/N was achieved on rigid substrates (SiO<sub>2</sub>/Si). In all cases, a thin Al buffer layer was deposited, immediately before AlN, without breaking the vacuum in the deposition chamber, in order to preserve the interface from contaminations that would obstruct the optimal atomic stratification with the desired [0001] growth axis. The piezoelectric behavior was thus correlated to the degree of texturing of the AlN layer through the evaluation of the XRD texturing coefficients and to the morphology by means of AFM analyses. We show that a high level of roughness introduced by the PEN substrate, coupled with the effect of the substrate on the piezoelectric coefficient, reduces the impact of the AlN texturing on the  $d_{33}$  values.

**#358 - FLEXIBLE NON-ENZYMATIC GLUCOSE SENSOR BASED ON LOW-COST NI NANOFOAM**

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Accurate and fast glucose sensing is of paramount importance in several key technology areas, such as health care, food industry and biotechnology. Most current commercial devices are typically based on enzymatic glucose detection, which usually suffers from poor stability of the immobilized glucose oxidase enzyme. Non-enzymatic glucose sensors have recently attracted great scientific attention as reliable, selective and fast glucose sensing (sensitivity of few  $\text{mA mM}^{-1} \text{cm}^{-2}$ ) can be achieved. The use of Ni as electrocatalyst for glucose biosensing takes advantage of the  $\text{Ni}^{2+}/\text{Ni}^{3+}$  red-ox shuttle which is capable of fast and effective glucose oxidation. Still, the preparation of high surface area nanostructured Nickel is still challenging, sometimes involving the use of high temperature, pressure and vacuum systems, as well as exotic substrates. Here we present a simple route for the preparation of high surface area Ni nanostructures which are used for low-cost fabrication of flexible (plastic substrate) glucose biosensors with high efficiency.

Ni nanostructures are obtained through room temperature chemical bath deposition involving Nickel sulfate, potassium persulfate and ammonia solution. FTO (Fluorine doped Tin oxide) covered glass or ITO (Indium Tin oxide) covered UPILEX plastic (50  $\mu\text{m}$  thick) were used as substrates. The synthesis created a highly porous film of intertwined NiO sheets (nanowalls, NWL) which, after forming gas annealing at 350°C converts into a packed ensemble of small (20 nm) Ni particles (nanof foam, NF). Scanning electron microscopy, X-ray Diffraction, temperature programmed reduction, BET surface area analyses, were used for chemical and structural characterization, while a VersaStat 4 potentiostat was used for voltammetry and chronoamperometry studies in a three electrodes set-up. The Ni NF electrode (both on plastic and glass substrates) was conditioned for glucose sensing by cyclic voltammetry (CV) between -0.1 and 0.8 V in 0.1 M NaOH solution. Chronoamperometry (current vs. time) analyses were carried out by monitoring changes in the amount of current increase with increase in glucose concentration of the 0.1 M NaOH electrolyte at 0.5 V vs SCE. The results show a linear response in the 10-700 mM glucose concentration and a sensitivity of  $3 \text{mA mM}^{-1} \text{cm}^{-2}$ . Long-term stability, high selectivity, fast response and excellent resistance to chloride ions were demonstrated.

**#359 - Recent advances in the integration of optical fibers and fiber-based sensors in nuclear environments**

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In this talk, the recent advances about the integration of optical fibers and fiber-based sensors in nuclear environments will be reviewed.

For operation in such harsh environments, fiber-based devices present key advantages compared to other technologies such as low weight, multiplexing capabilities, electromagnetic immunity... However, their integration remains limited by three degradation mechanisms that are radiation induced attenuation (RIA), radiation induced emission (RIE) and radiation induced refractive index changes (RIRIC). The amplitudes and kinetics of these changes are mainly driven by the nature, optical and structural properties of the point defects created by ionization of displacement damages in the amorphous pure or doped silica of the fiber core and cladding.

As a consequence, several intrinsic and extrinsic parameters influence the fiber or sensor radiation response such as the fiber composition, the irradiation characteristics (dose, dose rate), the temperature or operating wavelength. A survey about these parameters and their impact on RIA will be given at the conference together with guidelines for the selection of fibers for data transmission in major radiation environments (space, military, fusion or fission facilities)...

More recently, there is an increasing needs for fiber-based sensors using the fiber itself at the sensitive element to external parameters such as radiation dose, temperature, strain, pressure. These systems combined with reflectometry techniques authorize today to monitor these measurands with one meter spatial resolution over kilometers (Raman, Brillouin sensors) or millimeter resolution over tenths of meters (Rayleigh sensors) whereas punctual measurements are possible with Fiber Bragg Grating technology. Potential of these sensors for operation in the extreme conditions of the nuclear industry, nuclear waste storage and high energy physics facilities will be discussed.

**#360 - Large-area luminescent solar concentrators based on 'Stokes-shift-engineered' nanocrystals**

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Luminescent solar concentrators (LSCs) were proposed for the first time more than three decades ago as a cost-effective alternative to Si-based solar cells. They consist of semitransparent plastic slabs doped or coated with highly emissive chromophores which, after the absorption of the sunlight, emit long-wavelength photons. The luminescence is guided by total internal reflection to the waveguide edges, where it is converted into electricity by conventional PV cells installed along the slab perimeter. Thanks to their easy integration into active architectural elements, which enormously extends the surfaces exploitable for the light harvesting, LSCs are actually one of the most promising complement for the realizations of net zero-energy consumption buildings in highly-populate urban areas. However, despite a great flurry of activity in the field leading to a plethora of patents, the integration of LSCs in real-world applications is still hindered by the intrinsic limitation imposed by organic molecules and conventional quantum dots commonly used as emitters. In particular, reabsorption losses and a partial coverage of the solar radiation prevent the realization of large-area devices with suitable efficiency.

Recently we demonstrated two different strategies for realizing LSC with reduced absorption losses and high efficiency for dimension up to tens of centimeters, by employing both wavefunction engineered [Nature Photonics, 8, 392 (2014)] and ternary [patent application MI2015A000041] quantum dots (QDs). In the first case the active chromophores are CdSe/CdS QDs with a giant shell (responsible for the absorption) and a small core (responsible for the emission). In the second one, ZnS-coated CuInSe<sub>2-x</sub>S<sub>x</sub> QDs provide a Stokes-shifted emission due to deep intra-gap states associated with native defects. The feasibility of these approaches was proved by fabricating high-optical-quality nanocomposites embedding the selected QDs in polymethylmethacrylate or poly(lauryl-methacrylate) matrixes properly polymerized in order to preserve the optical properties of the emitters. In such a way, we obtained large-area, freestanding, colorless polymer slabs achieving an optical power efficiency of 3.2% without the assistance of back-reflectors. Monte-Carlo simulations show that, with few improvements of the QD photoluminescence quantum yield, high efficiency LSC as large as one square meter can be easily obtained opening the way for the fabrication of photovoltaic windows.

**#361 - Silicon carbide materials for photo-sensing applications: optical and structural characterization**

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Wide-bandgap semiconductors are widely used for applications in the field of optoelectronics and microelectronics. Among these, silicon carbide (SiC), both in its amorphous and crystalline form, is regarded a promising material due to its outstanding properties



in harsh environment [1]. Extreme thermal stability and large electric breakdown fields make it suitable for the development of high-temperature, high power, high-frequency applications and UV optoelectronic devices [1].

Crystalline SiC forms long range ordered structures and according to the possible stacking sequence along the crystallographic axis direction, it is characterized by many different polytypes, each one identified by their own featuring electrical and optical properties [2]. Among all the polytypes, the hexagonal structure 4H-SiC, has been studied as a proper material for optoelectronic applications [3]. Indeed, synthesis is mainly focused on 4H-SiC production because, regarding other polytypes, it has substantially higher carrier mobility, shallower dopant ionization energies and low intrinsic carrier concentration [4]; moreover, it is characterized by transparency to the visible spectrum, high sensitivity to photons and radiation-hardness [5].

In this work, we provide a detailed study of variously doped 4H-SiC properties for photo-sensing applications. In order to obtain information on defects, doping, and spatial uniformity of films, an accurate analysis by means of micro Raman spectroscopy and Raman mapping is performed. The films are also optically characterized using spectroscopic ellipsometry to determine optical and electro-optical parameters.

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### #362 - Proton beams Bragg peak imaging by LiF color centers-based photoluminescent detectors

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Lithium fluoride (LiF) is a well-known material for photonic applications [1] and dosimetry. LiF crystals and thin films have also been proposed and tested as high spatial resolution luminescent solid-state x-ray imaging detectors [2,3]. In recent years, the use of hadrons (i.e. protons and carbon ions) in oncological radiotherapy has seen a considerable expansion because of the excellent ballistic properties of heavy particles which lose most of their energy just at the end of their path in tissue, called Bragg peak, with a modest lateral diffusion and preserving the surrounding healthy organs during tumor irradiation.

Proton beams of 3, 7 and 11.6 MeV energy, produced by a linear accelerator at ENEA C.R. Frascati, were used to irradiate in a particular geometry LiF thin films thermally evaporated on silicon, inducing the formation of stable primary and aggregate color centers (CCs). In particular,  $F_2$  and  $F_3^+$  defects (two electrons bound to two and three anion vacancies, respectively) possess almost overlapping absorption bands, located at a wavelength of about 450 nm; under optical excitation in this spectral region they emit broad photoluminescence (PL) bands peaked at 678 nm and 541 nm, respectively.

By a standard fluorescence microscope, images of the top surface of the exposed LiF films allowed evaluating the Bragg peak position. The spectrally integrated PL emitted by radiation-induced  $F_2$  and  $F_3^+$  CCs, whose local concentrations are proportional to the energy deposited by protons in LiF [4], exhibits a strong increase at a distance from the edge of the film, which depends on the proton beam energy. As the PL signal is proportional to the local defects concentrations, this strong increase appears to be related to the Bragg peak position. At the investigated proton beam energies, the estimated distance between the film edge and the PL peak intensity is in satisfactory agreement with the simulations obtained by using The Stopping and Range of Ions in Matter (SRIM) software. These preliminary results strongly encourage the use of LiF thin films for advanced diagnostics of proton beams.

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### #363 - Structure and fluorescence mechanism of highly N-doped Carbon nanodots

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Carbon nanodots (CDs) are an emerging family of carbonaceous nanoparticles capable of an intense and tunable fluorescence in the visible. CDs can be synthesized by a variety of methods ranging from electrochemical oxidation of graphite to microwave-induced decomposition of organic molecules. CDs often consist in a crystalline core rich of  $sp^2$ -carbon, surrounded by an oxidized surface shell hosting a variety of polar groups which make CDs highly soluble in water. However, their structure and properties undergo notable variations depending on the synthesis method. For instance, CDs sometimes lack any crystalline order in the core, and their fluorescence sensibly depends on surface passivation. Apart from C, O and H, CDs are often surface-passivated or core-doped with Nitrogen, as a practical way to enhance their fluorescence quantum yield (QY). The strong fluorescence of CDs, combined with water solubility, versatile photochemical properties and low cost, has inspired several possible applications in light-emitting devices, sensing, solar energy harvesting and more, which are the subject of intense research. On the other hand, many questions remain open on the fundamental photo-physics of CDs, such as assigning their emission mechanism to transitions in the nanocrystalline core, to surface-localized electronic states or both.

We synthesized highly Nitrogen-doped CDs via a bottom-up procedure, and studied in detail their properties by HRTEM, AFM, XPS, FTIR, Raman, VIS/UV absorption and photoluminescence. Structural analysis via HRTEM, AFM and electron diffraction shows CDs to be sized  $\approx 3$  nm on average and, more importantly, to host a crystalline  $b\text{-C}_3\text{N}_4$  core, in contrast with the usual picture of CDs having an essentially graphitic structure. The surface of CDs hosts plentiful carboxylic and amide groups, as inferred from FTIR and XPS data. We find CDs to be strongly fluorescent in the visible, with large QYs and nanosecond decay lifetimes under VIS/near-UV excitations, the fingerprint of strongly dipole-allowed electronic transitions. The evidence that the emission color can be tuned by selecting the excitation wavelength implies a continuous distribution of fluorophores having inhomogeneously distributed electronic gaps. Temperature-dependent fluorescence data also reveal these fluorophores to be coupled to a vibrational mode of defined frequency. We finally attribute the fluorescence to electronic transitions essentially associated to their surface moieties.

#### **#364 - Rare Earth doped Y<sub>2</sub>SiO<sub>5</sub> characterization for Optical Stimulated Luminescence Dosimetry applications.**

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Rare Earths doped oxyorthosilicates, (RE<sub>2</sub>SiO<sub>5</sub>) are widely used as highly efficient and fast scintillators matrix for  $\gamma$ -ray detection. In the last decades Ce doped Y<sub>2</sub>SiO<sub>5</sub> (Ce:YSO) crystals, for example, renewed large scientific and technological interest in their properties as scintillator materials or phosphors. From these point of views, the crystal structure of pure yttrium oxyorthosilicates (YSO) needs to be free of structural defects in order to avoid unwelcome shallow or deep intragap energy levels that decreases light yield and can generates afterglow that further reduce the efficiency of the final devices. However in this work we focus on the possibility to control and use such carrier traps to engineer new devices for optical memory storage. The use of oxyorthosilicates as dosimeters for the high energies (MeV) is still an open topic of research and in recent years the properties of this material were compared with other hosts, like carbon doped Al<sub>2</sub>O<sub>3</sub>, especially in Optically Stimulated Luminescence Dosimetry (OSLD) measurements. Indeed, beside their stopping power, the energy and information storage properties of dosimetry materials were recently investigated in order to find the most promising host for OSLD measurements able to guarantee the right compromise between high sensitivity and high efficiency in dose reading coupled with a stopping power similar to human tissues. Taking into account these requests, new Rare Earth doped silicate nanoparticles, were grown by sol gel method and deeply characterized in comparison to Ce:YSO crystals. In this perspective, the optical and structural characterizations of YSO are presented and the effects of visible irradiation on the thermoluminescence measurements are discussed. Different trap levels are observed both in nitrogen atmosphere grown nanoparticles of YSO and silicate samples, and the selective effects of light irradiation show the feasibility, in the near future, of RE doped silicate crystals as promising OSL dosimeters.

#### **#365 - Bismuth and Erbium co-doped yttrium oxide for efficient photonics devices at 1.54 micron**

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In the last decades erbium-containing materials have been widely used as active media in large-scale communication systems, due to the fact that Er emission at 1.54 micron corresponds to a minimum of loss in silica optical fibers. However, in order to introduce it into active media for efficient silicon microphotonics devices, high Er contents are required but limited by the Er solid solubility, that leads to the formation of optically inactive Er metallic clusters. To overcome this limit we developed yttrium-erbium based compounds in which Er concentration can be modulated by Er ions replacement of Y ones in substitutional positions, thus avoiding the formation of Er clusters and increasing the Er content up to  $10^{22}$  Er/cm<sup>3</sup>. Moreover to further enhance the optical efficiency of the system, by increasing the Er excitation cross section, we introduced also a sensitizer that absorbs light more efficiently and transfers it to Er ions. As sensitizer we chose bismuth because, among the different oxidation states in which it can be stabilized, Bi<sup>3+</sup> is the most common and has an excitation cross section up to four orders of magnitude higher than the Er one. For this

purpose, we have synthesized (Bi+Er)-doped Y oxide with different Bi contents by ion implantation and magnetron co-sputtering. The Bi influence on structural and optical properties of the compound have been studied and will be widely discussed. In particular it has been found that  $\text{Bi}^{3+}$  ions in yttrium oxide can occupy two different lattice sites,  $\text{C}_2$  and  $\text{S}_6$ , having characteristic excitation bands in the ultraviolet region and emission bands in the green and blue range, respectively. By comparing the photoluminescence excitation spectra (PLE) of the Bi-doped and of the (Bi+Er)-doped yttrium oxide samples, it has been demonstrated that  $\text{Bi}^{3+}$  ions, in both lattice sites, can excite Er ions. The energy transfer efficiencies have been estimated by evaluating the reduction of Bi decay-time in presence of Er.

By comparing Er PL properties with and without Bi, we have also evaluated the Er effective excitation cross section through the Bi mediated process, that has been found to be three orders of magnitude higher than the Er direct excitation at 488 nm. The obtained value is the highest observed in silicon-compatible materials. Moreover, both the approaches of Er-based compounds to dissolve high Er contents and the use of an efficient sensitizer, such as Bi, have permitted to reach high Er optical efficiency at 1.54 micron. Therefore these results demonstrate the potential of Bi-doped Y-Er oxide as a novel and efficient material to be used as active medium for photonic applications.

### #366 - Enlightening the nature of Fermi level states of Al:ZnO films in a wide doping range

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Al-doped Zinc Oxide (AZO) is an attractive material as transparent conductive oxide with applications in photovoltaics, optoelectronic devices and plasmonics, due to its transparency ( $E_g=3.2$  eV), high carrier concentrations ( $\approx 10^{20}$   $\text{cm}^{-3}$ ) and a tunable plasma frequency in the near infrared [1,2]. Doping up to the solubility limit of ~4 at.% determines the appearance of occupied states at Fermi Level (FL), due to the occupation of conduction band (CB) states by electrons donated by Al, with the consequent shift of FL above the CB minimum that allows conduction while preserving transparency [3]. Some works investigate the possibility that structural/chemical defects in the AZO matrix can induce gap states in the vicinity of the Fermi level that would lead to infrared (IR) interband transitions [4,5].

In this work we integrate IR absorption and Hard X-ray Photoemission Spectroscopy (HAXPES) to determine the contribution of defects to the electronic structure and the exact nature of the electronic states at FL of AZO films in a wide doping range. In particular we focus on the modifications introduced by Al presence at FL and the possible existence of interband transitions in the infrared range. The population of CB with electrons donated by dopant is confirmed and we exclude the contribution of defects states, based on the absence of interband transitions at low doping. Then we elucidate the electronic structure of AZO doped above the solubility limit, where new states appear in the gap near the VB maximum. These states are related to defects introduced in the oxide, that reduce the number of free carriers and also their mobility, as theoretically predicted [3]. The defects determine a depopulation of the CB and an enlargement of the electronic bandgap. Furthermore the extended doping range allows to study the evolution of plasma frequency by means of optical absorption in parallel to the electronic structure evolution, to determine the plasmonic response of the material.

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**#367 - Hydrogenated Graphene**

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On SiC(0001), epitaxial graphene is obtained by sublimation of Si from the substrate. The graphene film is separated from the bulk by a carbon-rich buffer layer which in part covalently binds to the substrate. We report scanning tunneling microscopy (STM) studies of the buffer layer and of quasi-free-standing monolayer graphene (QFMLG) that is obtained by decoupling the buffer layer from the SiC(0001) substrate by means of hydrogen intercalation. Atomic resolution STM images of the buffer layer reveal that, within the periodic structural corrugation of this interfacial layer, the arrangement of atoms is topologically identical to that of graphene. After hydrogen intercalation, we show that the resulting QFMLG is relieved from the periodic corrugation and presents no detectable defect sites [1].

Reversible hydrogenation of graphene has been recently reported, and it was shown that hydrogenation opens a bandgap in graphene. We report on site-selective adsorption of atomic hydrogen on monolayer graphene grown on SiC(0001), and measure a band gap which increases with increasing hydrogen coverage. Therefore, hydrogenation allows for band-gap engineering in graphene. We also show that at low coverage hydrogen is found on convex areas of the graphene lattice. No hydrogen is detected on concave regions. These findings are in agreement with theoretical models which suggest that both binding energy and adsorption barrier can be tuned by controlling the local curvature of the graphene lattice. This curvature dependence combined with the known graphene flexibility may be exploited for storage and controlled release of hydrogen at room temperature, making it a valuable candidate for the implementation of hydrogen-storage devices [2].

Furthermore, we investigate the morphology of QFMLG formed at several temperatures by hydrogen intercalation and discuss its relationship with transport properties. Features corresponding to incomplete hydrogen intercalation at the graphene-substrate interface are observed by STM on QFMLG formed at 600 and 800°C. They contribute to carrier scattering as charged impurities. Voids in the SiC substrate and wrinkling of graphene appear at 1000°C, and they decrease the carrier mobility significantly [3].

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**#368 - Generating and probing quantum dots with single-atom precision**

*Stefan Foelsch (I) - Paul-Drude-Institut für Festkörperelektronik*

Quantum dots are often called “artificial atoms” because, like real atoms, they confine electrons to quantized states with discrete energies. This makes them promising candidates for technological applications in photonics, optoelectronics, and quantum information processing. The main obstacle in the fabrication of semiconductor quantum dots is to control their size, shape, and arrangement because usually they consist of hundreds or thousands of atoms, resulting in inevitable variations in their energy level structure. In this presentation, it will be shown that quantum dots with identical, deterministic sizes can be created in a scanning tunneling microscope one atom at a time. By using the lattice of a reconstructed indium arsenide surface to define the allowed atomic positions, the shape and location of the dots can be controlled with effectively zero error. The dots are assembled from positively charged indium atoms, leading to the electrostatic confinement of intrinsic surface-state electrons. The described approach enables to construct quantum-dot assemblies (quantum-dot “molecules”) whose quantum coupling has no intrinsic variation but can nonetheless be tuned over a wide range. Quantum dots with precisely defined wave functions and energy levels – as realized here – are also excellent candidates for studying the behavior of electrons in reduced dimensions, avoiding the disturbing effect of stochastic variations in size and shape.

**#369 - Single-plasmon blockade with metallic nanostructures**

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Localized surface plasmons in ultra-sub-wavelength metallic nanostructures are responsible for a significant enhancement of light-matter interaction [1-3]. As a consequence, nonlinear quantum effects can be amplified up to a point where the interaction energy between two single plasmons, in the true sense of single quanta of energy at the nanoscale, becomes comparable with the plasmon linewidth and the system becomes sensitive to single-plasmon scattering. This regime is characterized by the phenomenon of *single-plasmon blockade*, i.e., the inhibition of the absorption of a single plasmon due to the presence of another one, which mirrors in the field of quantum plasmonics the single-*photon*-blockade effect [4] that has been recently demonstrated in cavity-quantum-electrodynamics systems with groundbreaking experiments [5,6].

We discuss the quantization of surface plasmons on the basis of the quasinormal modes formalism [7], and we show that single-plasmon blockade can be realistically predicted for a plasmonic system made of a metallic nanodimer (e.g., in the bowtie configuration) with local infiltration or deposition of a nonlinear material with a sufficiently high third-order susceptibility in the

interstitial region of the dimer. Moreover, we show that single-plasmon blockade can be observed under pulsed excitation, overcoming possible experimental issues related to the plasmon short lifetime. Indeed, at variance from photonic systems, which typically rely on long-lifetime optical resonators, single-plasmon blockade in plasmonic systems could potentially provide an unprecedentedly ultra-fast source of quantum states of radiation, turning the short lifetimes of plasmons into an interesting technological resource.

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### #370 - Local strain and bandgap engineering in layered MoS<sub>2</sub>

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Graphene has represented in the past 10 years the most promising new material for a new generation of electronic devices and for the investigation of fundamental physics. The effective employment of graphene-based materials in low-energy electronics is however hindered by the difficulty of opening bandgap without affecting the mobility and the electronic properties.

New actors have however recently entered on the stage, in particular metal-transition dichalcogenides, as MoS<sub>2</sub> and similar compounds. Also these materials, like graphene, can be exfoliated to reach atomically thickness. In advantage, they present an intrinsic bandgap whose nature and size results to be highly sensitive to the number of layers and to external conditions (strain, pressure, electric fields, etc.).

In this talk we demonstrate the possibility to control at a local scale the electronic and optical properties by means of local strain.

Lattice corrugations are induced in few-layer MoS<sub>2</sub> samples by means of controlled delamination on an elastic substrate. Local strain is monitored through the phonon resonance energies in Raman spectroscopy, and the local direct bandgap is measured by

photoluminescence. The direct correlation between these features proves the feasibility to control the bandgap at a local scale by means a suitable pattern of strain.

To understand these results, we generalize a proper tight-binding model for MoS<sub>2</sub> under non-uniform conditions, accounting for the local modulation of the hopping integrals. Such analysis suggests a possible change between direct- to indirect-bandgap upon strain at a local scale, and a possible "funnel effect" in large wrinkles.

### #371 - Ballistic Transport at the Nanometric Inhomogeneities in Au/Nb:SrTiO<sub>3</sub> Resistive Switches

Andrea Gerbi - CNR-SPIN

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Nanometer-scale alterations of the Schottky barrier represent one of the microscopic mechanisms proposed to explain the resistance switching in transition-metal oxide cells. We report on novel Ballistic Electron Emission Microscopy (BEEM) experiments aimed to directly visualize and quantify the local inhomogeneities of the effective Schottky barrier height on Au/Nb:SrTiO<sub>3</sub> Schottky junctions dominated by interfacial resistance switching effects [1].

The low Schottky Barrier Height (SBH) regions observed in our BEEM data, can be associated to the electron transport through spatially-localized defects of nanometric size in the interfacial layer. The same value has been observed also for the ON state in the macroscopic current-voltage (I-V) curves of the device. Outside the nanometric regions with low SBH, most of the interface of the diode is dominated by a higher value of the Schottky barrier in good agreement with the value extracted by our I-V curves in air and with the SBH observed in the OFF state.

The voltage-dependent variation of the local barrier height of the nanometric patches could explain the non-ideal behaviour of the resistance switching effects [2].

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**#372 - Scanning probe microscopy study of CVD-grown graphene transferred to Au(111)**

Nicola Galvanetto - KU Leuven

Other Authors: Koen Schouteden (KU Leuven), Chundong Wang (Huazhong University of Science and Technology), Zhe li (KU Leuven), Chris Van Haesendonck (KU Leuven)

Graphene was grown by chemical vapor deposition (CVD) on copper films and transferred ex situ to atomically flat Au(111) films, after which the sample is annealed in ultra-high vacuum (UHV) prior to scanning tunneling microscopy (STM) investigation. STM imaging at low temperatures reveals large, clean and defect-free atomically flat areas that are separated by graphene wrinkles

and grain boundaries. In addition to the graphene atomic structure, the flat surface regions exhibit patterns with larger periodicity that can be interpreted as Moiré patterns formed by the atomic lattices of the graphene and the gold. Our findings show that the CVD-growth and ex situ transfer of graphene to atomically flat Au(111) surfaces allows to obtain clean and high-quality G/Au surfaces that are suitable for in situ deposition of, e.g., molecules and atoms, for UHV investigation purposes.

This approach may offer a higher degree of freedom in preparing bare and doped graphene on atomically flat surfaces compared to a full in situ approach.

**#373 - Flexible field effect transistors based on 2D semiconductors for electronics and sensing**

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Two-dimensional (2D) materials such as the widely known graphene (Gr) and the rising family of the transition metal dichalcogenides (TMDs) are ideal candidates for flexible electronics, thanks to their excellent electrical properties and their mechanical flexibility. In particular, due to its high carrier mobility ( $10^3$ - $10^4$   $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ ), Gr can be extremely advantageous both for high-frequency devices and for interconnects. Furthermore, thanks to some peculiar properties, such as the highest surface to volume ratio and the finite density of electronic states close to the Dirac point, Gr is extremely susceptible to charge transfer phenomena from the surrounding environments. This makes Gr membranes suitable for environmental sensing applications (gas, PH, humidity,...), provided proper functionalization is performed to promote the selectivity to specific analytes. The lack of a bandgap makes Gr field effect transistors (FETs) unsuitable for switching applications due to the poor on/off current ratio. On the contrary, TMDs such as  $\text{MoS}_2$  represent a reasonable compromise between a good mobility ( $\sim 200$   $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ ) and the presence of a band gap (1.2 - 1.8 eV, depending on the layer number) which makes possible a high current on/off ratio ( $>10^6$ ).

The realization of such systems on plastics (PEN, PET,...) represents a challenge, due to the limitations on the maximum processes temperatures ( $<100$  °C) and on the use of chemicals imposed by these substrates. In this work we will present innovative solutions developed for the integration of Gr-based electronic devices (back-gated FETs, resistors, capacitors) and sensing elements (pH sensor, temperature sensors...) on large area (150 mm) PEN foils. These include novel clean (metal contamination free) methods to transfer Gr grown by CVD on copper foils to the target substrates [1], as well as low temperature deposition of high-k dielectrics. A thermo-compression printing approach based on nanoimprint lithography has been also developed to integrate thin  $\text{MoS}_2$  flakes exfoliated from bulk molybdenite on this flexible platform for the fabrication of switching FETs.

The electrical properties of these devices have been extensively characterized, both by static I-V characterization and by nanoscale electrical analyses based on AFM. Their performances as flexible electronic devices have been evaluated after several bending cycles, and their environmental sensitivity was investigated as a function of the pH of liquid analytes or as a function of the environment temperature

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**#374 - Subsurface Pd enrichment in Ag-Pd nanoparticles**

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The silver-palladium system is of great interest for applications in catalysis, for example, in hydrogenation reactions with enhanced selectivity [1]. Ag and Pd are miscible in the bulk phase for all compositions, without formation of ordered phases, while in nanoparticles there is experimental evidence in favour of some Ag surface segregation. Global optimization studies on small Ag-Pd clusters showed that Ag prefers to segregate on the surface [2]. However, a systematic study of the equilibrium segregation profiles in Ag-Pd nanoparticles was still lacking.

In this work, we investigated the preferred chemical ordering in Ag-Pd nanoalloys by means of global optimization searches with the atomistic Gupta potential [3]. We considered three different fixed geometric structures at selected magic sizes: an fcc

truncated octahedron (TO) of 586 atoms, an icosahedron (Ih) of 561 atoms and a Marks decahedron (Dh) of 434 atoms. The results of the optimizations singled out a behaviour whose main features are common to all these geometric structures. As expected, an Ag surface enrichment is found, but more surprisingly, also a neat subsurface enrichment in Pd. Thus Ag-Pd nanoparticles prefer a three-shell chemical ordering pattern, in which the surface shell is strongly enriched in Ag, the subsurface shell is strongly enriched in Pd, and the inner part of the nanoparticle is rather weakly enriched in Pd. This behaviour can be rationalized in terms of preferred sites for single impurities, and is more pronounced in fcc nanoparticles, because in Ih and Dh nanoparticles the inner sites in fivefold symmetry axes are quite favourable for Pd inclusions.

We have tested the dependence of these results from the temperature, by means of Montecarlo simulations. It came out that the subsurface Pd enrichment slowly decreases with temperature, but it is still significant well above room temperature (up to 800 K).

Furthermore, we compared the degree of subsurface enrichment we found in nanoalloys with the theoretical enrichment in bulk systems, that we obtained using the multilayer thermodynamic model developed by Strohl and King [4]. This comparison highlighted a stronger effect for nano-systems. This can be explained by the non-negligible amount of sub-edges and sub-vertexes sites, that are the most favourable for Pd inclusions.

These findings can be relevant to the understanding of the catalytic activity of Ag-Pd nanoparticles, especially for those reactions for which the role of subsurface sites is important.

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### #375 - Ultra-low contact resistance in graphene devices

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Two-dimensional materials, such as graphene, MoS<sub>2</sub> or WSe<sub>2</sub>, represent a new paradigm in thin-film transistor technology, providing also the opportunity for new device concepts. Graphene is one of the possible contenders in high-frequency electronics, mainly due to its high charge carrier mobility and velocity saturation, which exceed that of conventional high-mobility semiconductors (III-V or SiGe). Scalable production techniques, such as chemical vapor deposition (CVD), can now deliver graphene on a large scale which is interesting from the industrial point of view. However, fabrication of graphene field-effect transistors (GFETs) need further development if graphene is to compete with established semiconductor technologies. One of the main parameters degrading high-frequency response of GFETs is contact resistance which should be reduced below Ohm $\mu$ m to reach that of conventional high-frequency transistors.

Here we demonstrate graphene/metal contacts with a typical contact resistance of 80 Ohm $\mu$ m at the Dirac point. The contact resistance was determined by transmission line measurements (TLMs) at room temperature. The low contact resistance was obtained by etching holes in CVD-grown graphene before the deposition of contacts. This increases the contact edge with metal contacts deposited on top and therefore the injection of carriers at the graphene edges. Pure Au contacts were used without any adhesion layer or thermal treatment. We performed measurements of two-probe resistances in a typical graphene TLM test device fabricated on a conventional SiO<sub>2</sub> (300 nm)/Si substrate. The lowest contact resistance was 72 Ohm $\mu$ m. Such ultra-low contact resistance is comparable to that of InP THz transistors and provides a viable route to high-frequency GFETs.

**#376 - Computer simulations of gel-formation via catalytic reactions***Walter Kob (I) - University of Montpellier**Other Authors: Virginie Hugouvieux (INRA, UMR1083, University of Montpellier and Montpellier SupAgro, Montpellier, France)*

Certain biopolymers transform into a gel by a catalytic reaction in which a freely moving catalyst transforms the monomers of the polymer into a multi-functional point. These points stick to each other and make that the polymer sol slowly transforms into a gel. Important examples for such systems occur in plant cell walls where polysaccharides (pectins) can undergo gelation due to the presence of an enzyme (pectin methylesterase).

In this talk I will present a simple model that describes this catalytic reaction. Using large scale computer simulations to probe the properties of this model we have investigated how the polymer sol transforms into the gel. In particular we have studied how the density of the polymers, the concentration of catalysts, and temperature influence the properties of the system at long times. We find that, depending on the choice of these parameters, the catalytic reaction can lead to a phase separation of the polymer solution, a heterogeneous gel, or a relatively homogeneous random network, and discuss the properties of these different structures.

**#377 - A neural network potential for water: Effect of van der Waals interactions on the thermodynamics, structure and dynamics of water***Christoph Dellago (I) - University of Vienna**Other Authors: Andreas Singraber (University of Vienna), Tobias Morawietz (University of Bochum), Jörg Behler (University of Bochum)*

Realistic molecular dynamics simulations of condensed matter systems require the accurate calculation of the forces acting on atoms. While ab initio methods can be used for this purpose, their high computational cost often precludes their application to large systems and/or long simulation times. For instance, ab initio simulations of water are currently limited to roughly one hundred molecules that can be followed by about 100 picoseconds. Here, we report on a neural network potential we have recently developed for liquid and solid water. This approach, in which reference data obtained from electronic structure calculations are used to train a neural network for the prediction of energies and force, yields the accuracy of ab initio simulations at a fraction of their cost. Using neural network potentials obtained for several density functionals with and without van der Waals corrections, we simulated the coexistence of water and ice, finding that the inclusion of van der Waals forces is crucial for an accurate prediction of the freezing point. These weak forces determine the flexibility of the hydrogen bond network and are also responsible for the density maximum of liquid water.

**#378 - Bridging and depletion mechanisms in colloid-colloid effective interactions: A reentrant phase diagram?***Riccardo Fantoni - Universita' Ca' Foscari di Venezia**Other Authors: Andres Santos (Departamento de Física and Instituto de Computación Científica Avanzada (ICCAEx), Universidad de Extremadura, E-06071 Badajoz, Spain), Achille Giacometti (Dipartimento di Scienze Molecolari e Nanosistemi, Università Ca' Foscari Venezia, Calle Larga S. Marta DD2137, I-30123 Venezia, Italy)*

A general class of nonadditive sticky-hard-sphere binary mixtures, where small and large spheres represent the solvent and the solute, respectively, is introduced. The solute-solute and solvent-solvent interactions are of hard-sphere type, while the solute-solvent interactions are of sticky-hard-sphere type with tunable degrees of size nonadditivity and stickiness. Two particular and complementary limits are studied using analytical and semi-analytical tools. The first case is characterized by zero nonadditivity, lending itself to a Percus–Yevick approximate solution from which the impact of stickiness on the spinodal curves and on the effective solute-solute potential is analyzed. In the opposite nonadditive case, the solvent-solvent diameter is zero and the model can then be reckoned as an extension of the well-known Asakura–Oosawa model with additional sticky solute-solvent interaction. This latter model has the property that its exact effective one-component problem involves only solute-solute pair potentials for size ratios such that a solvent particle fits inside the interstitial region of three touching solutes. In particular, we explicitly identify the three competing physical mechanisms (depletion, pulling, and bridging) giving rise to the effective interaction. Some remarks on the phase diagram of these two complementary models are also addressed through the use of the Noro–Frenkel criterion and a first-order perturbation analysis. Our findings suggest reentrance of the fluid-fluid instability as solvent density (in the first model) or adhesion (in the second model) is varied. Some perspectives in terms



of the interpretation of recent experimental studies of microgels adsorbed onto large polystyrene particles are discussed.

### #379 - Physical and chemical constraints on semi-dilute polymer solutions

Barbara Capone - University of Vienna

Other Authors: Emanuela Bianchi (2), Lorenzo Rovigatti (1), Ivan Coluzza (1), Christos Likos (1) (1) Computational Physics, University of Vienna, Austria (2) Institute of Theoretical Physics, Vienna University of Technology, Vienna, Austria

Multi-scale molecular modeling in polymer physics is a very important tool to access regions in the phase space where the inhomogeneity of polymers in solution does not allow pure theoretical approaches, and simulations become prohibitive.

Different levels of coarse graining allow to describe different local or global properties of the system, with qualitative and quantitative predictive power. In this talk I will present different multi-scale molecular modeling applied to various systems: concentrated solutions of unknotted and non-concatenated ring polymers in good solvent conditions and block copolymer with different physical or chemical constraints.

I will show how a detailed \textit{first principles} coarse-graining strategy based on analytically determined effective pair potentials between subsegments in the polymeric chains, computed at zero density, allows to quantitatively reproduce single molecule and solution properties of a system with well-defined physical constraints, but how dealing with temperature effects increases the difficulty of the description.

### #380 - Soft self-assembled nanoparticles with temperature-dependent properties

Lorenzo Rovigatti - University of Vienna

Other Authors: Barbara Capone (Faculty of Physics, University of Vienna), Christos N. Likos (Faculty of Physics, University of Vienna)

The fabrication of versatile building blocks that are reliably self-assemble into desired ordered and disordered phases is amongst the hottest topics in nowadays material science. To this scope, more or less complex microscopic units, aimed at assembling the target phases, have been thought, designed, investigated and built. Such a path usually requires laborious fabrication techniques, especially when a specific functionalisation of the building blocks is required.

Telechelic Star Polymers, that are star polymers made of a number  $f$  of di-block copolymers made of solvophobic and solvophilic monomers grafted on a central anchoring point, have been shown to spontaneously self-assemble into soft patchy particles, i.e. particles with attractive spots (patches) on the surface.

Here we show that the tunability of such a system can be widely extended by controlling the physical/chemical parameters of the solution. On top of the athermal self-assembly behaviour, that only depends on the number of arms and/or on the ratio of solvophobic to solvophilic monomers, it is hence possible to reliably change the number and size of the attractive patches by means of changes in temperature and/or solvent quality. This allows to change the mesoscopic self-assembly behaviour without modifying the microscopic constituents.

Interestingly, we also demonstrate that diverse combinations of the parameters can generate stars with the same number of patches but different radial and angular stiffness. This mechanism could provide a neat way of further fine-tuning the elastic properties of the supramolecular network without changing its topology.

### #381 - Chiral Self-assembly of Helical Particles

Achille Giacometti - Universita' Ca' Foscari Venezia

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The shape of the building blocks plays a crucial role in mediating and directing self-assembly towards the desired architectures [1,2]. Among the different shapes, helix has a unique position. Helical structures are ubiquitous in nature and a helical shape is exhibited by the most important biopolymers like polynucleotides, polypeptides and polysaccharides, and also by cellular organelles like flagella. Helical nanoparticles can self-assemble into chiral superstructures, which can have a variety of applications, e.g. as photonic metamaterials [3,4]. Despite their abundance in nature, a clear understanding of the phase behaviour of helical particles is still lacking. \ We have recently undertaken an extensive investigation of the phase diagram of hard helical particles, modelled as chains of

hard spheres [5,6,7] using Monte Carlo simulations and density functional theory. We have found a variety of chiral phases with liquid crystal order, most of which specific to the helical shape. These feature a new kind of screw-like order, characterised by roto-translational coupling, of which there is experimental evidence in suspensions of helical flagella [8].

We have obtained the complete phase diagram, as a function of the helix morphology. This includes conventional nematic and cholesteric phases, and other chiral phases with different degrees of hexagonal ordering, as well as possible chiral crystal structures. The possibility of engineering self-assembly of nanomaterials through a tuning of the chirality of the building block nanoparticles is discussed.

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### #382 - Interplay between geometrical constraints and alphabet size in the design of patchy polymers

Chiara Cardelli - *Computational Physics Group, University of Vienna*

Other Authors: Valentino Bianco (*Computational Physics Group University of Vienna*), Ivan Coluzza (*Computational Physics Group University of Vienna*)

Patchy polymers can be designed to self-assemble into specific structures.

The aim of polymer design is to find a sequence of particles along the chain that will fold into a target structure, according to a given "alphabet" of interacting particles [1-2]. The alphabet size and the geometrical constraint introduced by the patches affects the designability of the polymer. Here we study, via MC simulation, how the alphabet size and the number of patches i) determine the phase space of the sequences and ii) make the polymer designable.

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### #383 - Janus-like magnetic colloids in theory and simulations.

Sofia Kantorovich - *University of Vienna, Ural federal University*

Other Authors: Ekaterina Novak (*Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia*)

Understanding self-assembly of interacting colloidal particles is a key to controlling the pattern formation at the scales from atomic to macroscopic sizes. There are various types of interactions that can lead to the colloidal aggregation: magnetic or electrostatic forces, solvophobicity of the building blocks, etc. In this contribution we present our recent results on theoretical analysis and computer simulations of Janus-like dipolar particles and colloids with dipolar caps. The experimental prototypes for both types of

colloids are the magnetic Janus particles (*Soft Matter*, 2013,9, 9174-9181) and magnetically capped colloids (*Physical Review E* 77 (3), 031407). To describe the basic features of the Janus-type and capped magnetic colloids, we put forward a simple model of a spherical particle with a dipole moment shifted outwards from the centre and oriented perpendicular or parallel to the particle radius. We investigate both the ground states of small clusters and the behaviour of bigger systems at various temperatures. We show how the shift of the dipoles affects the ground states and, as a consequence, leads to a different microscopic behaviour in the situation when the thermal fluctuations are finite. For magnetic Janus particles we show that the topology of small clusters in the ground state is compact and the chain configurations are not anymore energetically advantageous. This strongly affects the response of the Janus-like particle systems to an external magnetic field at finite temperatures (*J Phys Condens Matter*, 2015 Jun 17;27(23):234102). As for the capped colloids, we show that experimentally observed metastable states occur due to the cap extension, and one needs to introduce a more accurate model for the cap description than that of a single dipole shifted outwards from the particle centre of mass. We extensively compare our prediction to the experimental data.

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**#384 - Molecular Materials for Artificial Photosynthesis**

Marcella Bonchio (I) - University of Padova and ITM-CNR UoS of Padova

Natural Photosynthesis has emerged from the adaptive evolution of light-activated molecular machineries, shaped and optimized by the dynamic assembly of proteins, pigments and metal-cofactors. Man-made photosynthetic systems lie far behind the natural paradigm, being largely based on covalent strategies, plagued by unproductive losses and unable to catch up with the up-hill water oxidation hurdle. The functional core of oxygenic photosynthesis, a unique  $Mn_4O_5Ca$  cluster (PSII-OEC), is in charge of catalytic water oxidation via a multi-redox manifold; evolving through five electronic states within the protein matrix. The synthetic transposition of such catalytic cycle is the expected turning point for artificial photosynthesis. We present herein a bio-inspired approach to photocatalytic water splitting by multi-metal cores, whose coordination sphere is tuned by the ligand set, including polyoxometalates. Our results address the tailored construction of functional interfaces, shaped at the molecular level and evolved to hybrid nano-structures.[1-5].

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**#385 - Scanning (Photo-) Electron Microscopy and Spectroscopy of Working Devices under Realistic Conditions**

Andrei Kolmakov (I) - Center for Nanoscale Science and Technology, NIST

Scanning (Photo-) Electron Microscopy and Spectroscopy of Working Devices under Realistic Conditions The processes taking place at the surfaces and at interfaces of micro-(nano-) devices such as sensors, memristors, batteries etc., determine their ionic and electronic transport properties and eventually a device overall performance. Electron and photoelectron microscopy in conjunction with surface sensitive electron spectroscopy are ideal tools to probe these properties. In this report, we implement recent developments in ambient pressure electron microscopy and spectroscopy to access the interplay between interfacial and transport properties of individual nanodevices operating under realistic conditions. In particular, electrochemical processes such as metal plating /intercalation from liquid electrolyte can now be probed in real time using ambient pressure XPS. Similarly, correlative measurements of the electron transport and surface chemistry of operating MEMS metal oxide sensor model device relate the conductance changes with formation of the specific surface groups upon redox reaction. The perspectives of the device characterization in operando mode and under real world pressures and temperatures will be outlined.

**#386 - First Principle Modelling of Structural, Optical and Charge Generation Properties of Dye/TiO<sub>2</sub> Heterointerfaces for Solar Energy and Solar Fuels**

Mariachiara Pastore (I) - CNR-ISTM

Other Authors: Filippo De Angelis (CNR-ISTM, Via Elce di Sotto, 8 06123 Perugia (Italy))

Within today's global challenge to exploit solar energy for a sustainable development, Dye-Sensitized Solar Cells (DSCs) and Solar Photocatalytic Cells (SPCs) offer the promise of low-cost sunlight conversion and storage.<sup>1</sup> In the last decade, theoretical and computational chemistry has started to play a prominent role in the development of higher efficient devices by helping the elucidation of the basic devices functioning mechanisms.<sup>2</sup> The fundamental information currently amenable to simulations are the dye geometrical structures, ground state oxidation potential, optical absorption spectra and excited state oxidation potential; and the semiconductor conduction band energy and/or density of states and its band gap. For the interface description, one needs to calculate the dye/catalyst adsorption modes onto the semiconductor, the nature and localization of the dye@semiconductor excited states and the energy level alignment at the dye/semiconductor heterointerface. We will critically address the potential and limitations of current DFT and TDDFT computational methods to model DSCs. While Ruthenium dyes are accurately modeled by standard DFT approaches, for highly conjugated organic dyes, characterized by strong charge transfer excited states, specifically tailored exchange-correlation functionals are needed, to overcome the complete neglecting of excited state density relaxation effects.<sup>3</sup> As matter of fact, currently available DFT/TDDFT methods, however, are not capable to deliver at the same time a balanced description of the dye@TiO<sub>2</sub> excited states and of the alignment of the dye excited states with the semiconductor manifold of unoccupied states. Finally we will present the basic methodology and selected applications of computational modeling of dye/TiO<sub>2</sub> interfaces in DSCs and SPCs.<sup>4,5</sup>

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**#387 - High Temperature Solar Cells based on Defect Engineered Diamond**

Paolo Calvani - CNR-ISM

Other Authors: Alessandro Bellucci (CNR-ISM, Area della Ricerca di Roma 1, Via Salaria km 29.300, Monterotondo Scalo (RM), Italy) Marco Girolami (CNR-ISM, Area della Ricerca di Roma 1, Via Salaria km 29.300, Monterotondo Scalo (RM), Italy) Daniele Maria Trucchi (CNR-ISM, Area della Ricerca di Roma 1, Via Salaria km 29.300, Monterotondo Scalo (RM), Italy)

Photon-enhanced Thermionic Emission (PETE) is a novel and very attractive concept for the exploitation of concentrated solar radiation with a promising conversion efficiency higher than 50%. PETE converters rely on the concept that engineered semiconductor structures can obtain a thermionic emission significantly enhanced by hot electrons generated by photons with sufficient energy to produce charge couples and sustained with the high temperatures induced by the absorption of photons with lower energy (i.e. IR. III-V semiconductors have been already used for the fabrication of a "proof-of-concept", but their unstable high temperature operations and the intrinsic high work-function are limiting conditions.

We propose a radically new and efficient PETE cathode based on surface-hydrogenated chemical vapour deposited (CVD) diamond, one of the few semiconductors to show negative electron affinity and a work function as low as 1.7 eV if nitrogen-doped. This characteristics assure an efficient thermionic emission at moderate temperatures (up to 780 °C). CVD diamond is transparent to solar radiation due to its wide bandgap of 5.47 eV, so advanced and novel techniques are needed for preparing an efficient sunlight absorbing diamond. Surface texturing by fs-laser, boron-implantation, buried graphitic contact structures and other technological steps allow the fabrication of an innovative defect engineered diamond cathode to be efficiently exploited for the conversion of concentrated solar light.

**#388 - Ab initio calculations of CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> degradation mechanisms in vacuum**

Ioannis Deretzis - Institute for Microelectronics and Microsystems (CNR-IMM)

Other Authors: Alessandra Alberti (CNR-IMM), Giovanna Pellegrino (CNR-IMM), Emanuele Smecca (CNR-IMM), Antonino La Magna (CNR-IMM)

Lead methylammonium tri-iodide (CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>) is a hybrid perovskite material with excellent light conversion efficiency that, however, suffers from fast degradation rates and structural instability. Here we study the mechanisms of CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> degradation and its transformation to PbI<sub>2</sub> by means of the density functional theory. We particularly focus on possible degradation mechanisms that go beyond the catalytic reaction with H<sub>2</sub>O. We argue that even in the absence of humidity, a disintegration of the perovskite structure can take place through the statistical formation of molecular defects with a non-ionic character, whose volatility at surfaces should break the thermodynamic defect equilibria. We finally discuss the strategies that can limit such phenomenon and subsequently prolong the lifetime of the material.

**#389 - Effects of bias stress on dye sensitized solar cell performance**

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Dye-sensitized solar cells (DSSCs) are promising third generation photovoltaic devices given their potential low cost and high efficiency. Some factors still affect the DSSC performance, such structure of electrodes, electrolyte compositions, nature of the sensitizers, issues of power conversion efficiency stability under prolonged electrical stresses, etc. In this work we discuss a technique based on electrical stresses which allows to improve DSSC performance and mitigate the above mentioned instability problems. We have investigated the effects of forward and reverse DC bias stress as a function of time, voltage, and illumination level in the DSSCs sensitized with the N719 Ruthenium complex based dye. We demonstrate that all the major solar cell performance parameters, i.e., open circuit voltage ( $V_{oc}$ ), short circuit current ( $I_{sc}$ ), series resistance ( $R_{oc}$ ), fill factor (FF), and power conversion efficiency are strongly influenced by the stress conditions and we show clear reversibility of the parameters on the stress type. We discuss the effect of temperature, bias level, and illumination intensity, and type of electrolyte and discuss possible causes of such effects. Our study reveals that by proper device biasing, the DSSCs noticeably improve in terms of efficiency and long-term stability.\*

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**#390 - Spontaneous knotting of DNA and other biomolecules: dynamical and functional aspects.***Cristian Micheletti (I) - SISSA**Other Authors: Marco Di Stefano (Univ. Barcelona), Davide Marenduzzo (Edinburgh Univ.), Henri Orland (CEA Saclay), Enzo Orlandini (Univ. Padova), Guido Polles (SISSA), Angelo Rosa (SISSA), Summers, De Witt (Florida State Univ.), Luca Tubiana (Wien Univ.)*

By using both coarse-grained models and bioinformatics approaches, we shall address a few prototypical examples of the intriguing implications of entanglement and knotting on the functional, mechanical and folding properties of various types of biomolecules. In particular, we shall discuss the kinetics of spontaneous knotting of long ssDNA chains and examine the "topological friction" accompanying their translocation through nanopores equivalent to those used in nanopore sequencing techniques. The broader implications for the ejection of knotted DNA out of viral capsids will also be discussed.

The material presented is based on the following publications:

- C. Micheletti et al. "Absence of knots in known RNA structures", PNAS, 2015, 112, 2052-2057
- G. Polles et al. "Self-assembling knots of controlled topology", Nature Commun., 2015, 6, art no. 6423
- D. Marenduzzo et al. "Topological friction strongly affects viral DNA ejection", PNAS, 2013, 110 20081- 20086
- L. Tubiana et al. "Spontaneous knotting and unknotting of flexible linear polymers: equilibrium and kinetic aspects", Macromol., 2013, 46 3669-3678
- A. Rosa et al. "Topological jamming of spontaneously knotted polyelectrolyte chains driven through a nanopore", PRL, 2012, 109 , 118301

**#391 - A fluctuation theorem for ligand binding***Felix Ritort (I) - Universitat de Barcelona/Facultat de Fisica/Small Biosystems Lab**Other Authors: Joan Camunas and Anna Alemany, Universitat de Barcelona, Facultat de Fisica, Small Biosystems Lab*

Intermolecular binding reactions drive a myriad of processes central to molecular biology such as gene regulation, recombination, ribosome assembly and immune response. We introduce a novel fluctuation theorem for ligand binding to measure binding energies of biomolecular reactions at the single-molecule level. We investigate single oligonucleotides, DNA restriction enzymes, and small ligands binding to DNA hairpins in single-molecule pulling experiments. Binding energies are directly measured as a function of ligand concentration providing a direct experimental verification of the law of mass action both for highly specific interactions and non-specific binding to multiple DNA sites. The possibility of monitoring single binding modes one at a time in single molecule experiments, in combination with the fluctuation theorem for ligand binding, makes now possible to determine the energetics of complex multimolecular assemblies with unprecedented reliability and accuracy

**#392 - Investigating drug resistance using molecular simulation***Carlioni Paolo (I) - Forschungszentrum Jülich, Germany*

The abstract will follow

**#393 - Binding of amino acids and peptides to gold surfaces***Stefano Corni - Centro S3, CNR Istituto Nanoscienze*

The interaction between proteins/peptides and inorganic surfaces and nanoparticles is crucial nanobiotechnology. On one hand, nanoparticles that contacts biosystems are readily covered by some of the proteins expressed by such biosystems. The resulting biological identity of the nanoparticle is then determined by which proteins bind, their orientation and possible structural changes [1]. Nanoparticles and surfaces are also known to affect the rate of protein/peptide fibrillation, i.e., the process leading to amyloid aggregates [2]. On the other hand, peptides able to recognize surfaces are promising building blocks for self-assembling of complex structures at the nanoscale [3]. Binding affinities (i.e., adsorption free energies) are crucial quantities in all these applications, both to quantify the relative propensity to bind and to provide microscopic interpretation to such complex binding phenomena. In particular, the way the internal free energy landscape of a peptide is modified by the interaction with a nanoparticle or a surface determines the stable conformations at the surface, and also the barriers separating such stable conformations (i.e., the kinetics of the conformational changes) [4].

In this contribution, atomistic calculations of binding of amino acids and peptides to gold surfaces in explicit water will be presented and discussed. These calculations rely on the force fields developed by our group [5], and exploit various enhanced sampling methods. These simulations provide relevant insights into the relative binding propensity of single amino acids, the nature of polypeptide conformational changes upon binding and the role of the gold hydration layer.

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### #394 - Controlling the motion of knots on tensioned polymers

Luca Tubiana - University of Vienna

Other Authors: Raffaello Potestio, Max Planck Institute for Polymer Research Mainz - Germany, Marco Di Stefano Centro Nacional de Análisis Genómico (CNAG) Barcelona - Spain, Massimiliano Di Ventra University of California San Diego (CA) - USA, Cristian Micheletti, SISSA-ISAS Trieste - Italy

Topological entanglement is an ubiquitous feature of many biological as well as artificial polymers. While the equilibrium properties of entangled chains have been the subject of several studies, the characterization of knot dynamics remains relatively unexplored. In this talk, we report computational results on two different meanings of affecting the motion of a knot on a tensioned polymer. Specifically, we show that i) external DC and AC electric fields acting longitudinally on a knotted dsDNA polymer can drive the knot along the chain and ii) that the onset of transverse waves on a flexible chain, caused by the mechanical driving of one end of the chain, traps the knot in spatially localized states, effectively discretizing the motion of the knot along the chain.

### #395 - Knotting and Unknotting Dynamics of DNA Strands in Nanochannels

Antonio Suma - SISSA - Scuola Internazionale Superiore di Studi Avanzati

Other Authors: Enzo Orlandini (Dipartimento di Fisica, Sezione CNISM, and Università di Padova, via Marzolo 8, I-35131 Padova, Italy), Cristian Micheletti (SISSA, International School for Advanced Studies, via Bonomea 265, I-34136 Trieste, Italy)

I will report on the theoretical characterization of the typical mechanisms governing the spontaneous tying, untying and the dynamical evolution of knots in coarse-grained models of DNA chains confined in nanochannels. Earlier studies address the knotting properties of DNA chains of  $L_c = 3.6\mu\text{m}$  confined in channels of different width,  $D$ , in the 50 – 300nm range[1]. It was thus established that knots typically originate from deep looping and back-foldings of the chain ends, and upon lowering  $D$ , backfoldings become shallower and rarer and the lifetime of knots decreases while that of unknots increases. Here, instead, I discuss how these mechanisms depend on the chain contour length,  $L_c$ , at a fixed channel width 56nm, corresponding to the onset of the Odijk scaling regime where chain backfoldings and hence knots are disfavoured but not suppressed altogether. In this case, the lifetime of knots grows significantly with  $L_c$ , while that of unknots varies to a lesser extent, as the lifetime of unknots is mostly controlled by backfoldings events at the chain ends, which is largely independent of  $L_c$ , while that of knots is controlled by how farther they can travel along the chain before being untied[2]. The observed interplay of knots and unknots lifetimes underpins the growth of the equilibrium knotting probability of longer and longer chains at fixed channel confinement. This results can aid the design of nanochannels capable of harnessing the self-knotting dynamics to quench or relax the DNA topological state as desired.

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### #396 - SPECTRUS: a dimensionality reduction approach for identifying dynamical domains in protein complexes from limited structural datasets

Luca Ponzoni - SISSA

Other Authors: Guido Polles (SISSA), Vincenzo Carnevale (Temple University, Philadelphia), Cristian Micheletti (SISSA)

Large-scale movements in proteins or protein complexes often arise from the relative displacements of only few quasi-rigid domains. Developing computational strategies for identifying such domains from limited sets of alternative conformers can help unveil the functionally-oriented protein mechanics. A natural way to inspect the internal rigidity of a protein is to look at the distance fluctuations between pairs of neighboring amino acids throughout a set of relevant conformations, which provide a straightforward measure of the local flexibility. The matrix of all distance fluctuations is then used for grouping amino acids into domains, by means of various clustering techniques. One common obstacle towards this goal is the dependence of the domain identification on the clustering methods used for partitioning, which are in general strongly affected by the scarcity of available data. A further challenge is the introduction of objective criteria for establishing the correct number of quasi-rigid domains.

We present a novel domain-decomposition method, named SPECTRUS, which can overcome both obstacles. The method takes as input the matrix of amino acids pairwise distance fluctuations and uses the Laplacian spectral projection to optimally expose the innate clustering of the amino acids into quasi-rigid domains, thus making their

identification practically independent of the chosen clustering scheme. Because of this robustness, SPECTRUS performs equally well when using distance fluctuation matrices computed from thousands of conformers sampled by extensive MD simulations, as well as just a pair of alternative crystal structures, or even a single conformer used as a reference structure for an elastic network model. Furthermore, we introduce a quality score that allows for an easier identification of the optimal number of domains, based on a measure of statistical significance of a given clustering compared to a random reference case.

The domain decomposition method was validated and applied to various systems of very different size, including monomeric globular proteins, multimeric ion channels and viral capsids. For the validation cases, the identified quasi-rigid domains are in excellent accord with those identified from supervised analysis of experimental or MD data. In the more challenging contexts where no prior indications of dynamical domains exist, the returned subdivision provide considerable insight into the functional dynamics of the biomolecules of interest.

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**#397 - Anomalous behavior of a driven tracer in a crowded environment***Olivier Benichou (I) - CNRS, UPMC*

We study a minimal model of active transport in a dense environment. We consider a discrete system in which a tracer particle performs a biased random walk in a bath of particles performing symmetric random walks with exclusion interactions. In confined geometries and in the high-density limit, an analytical calculation of the fluctuations of the tracer particle position predicts a long-lived superdiffusive regime. We show that this observation is associated to a velocity anomaly in quasi-one-dimensional systems (such as stripes or capillaries): the velocity of the tracer particle displays a long plateau before reaching an ultimate lower value. Finally, we study the case of one-dimensional systems, which is related to the well-known single-file diffusion.

**#398 - Non-normalizable densities for strong anomalous diffusion***Eli Barkai (I) - Bar Ilan University*

*Other Authors: Adi Rabenshtok<sup>1</sup>, Sergey Denisov<sup>2</sup>, Peter Hänggi<sup>2</sup> 1. Phys. Dept., Bar Ilan University, Israel 2. Phys. Dept, Augsburg University, Augsburg, Germany.*

Strong anomalous diffusion, where

$$\langle |x(t)|^q \rangle \sim t^{q\nu(q)}$$

with a nonlinear spectrum

$$\nu(q) \neq \text{const},$$

is wide spread and has been found in various nonlinear dynamical systems and experiments on active transport in living cells. Using a stochastic approach we show [1] how this phenomena is related to infinite covariant densities, i.e., the asymptotic states of these systems are described by non-normalizable distribution functions. Our work shows that the concept of infinite covariant densities plays an important role in the statistical description of open systems exhibiting multi-fractal anomalous diffusion, as it is complementary to the central limit theorem.

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**#399 - Anomalous fluctuations in nonlinear oscillator chains***Stefano Lepri (I) - Consiglio Nazionale delle Ricerche - Istituto dei sistemi complessi*

One-dimensional lattices of nonlinear oscillators often display anomalous energy diffusion and transport. This leads to a breakdown of macroscopic transport relations like e.g. the Fourier law. Recently, it has been argued that such anomalous fluctuations generically belongs to the universality class of the (seemingly unrelated) Kardar-Parisi-Zhang equation. We will present some simulation data that support this predictions.

**#400 - Superdiffusion and Transport in Lévy-like quenched disorder***Raffaella Burioni - Università di Parma*

*Other Authors: E. Ubaldi (Università di Parma), A. Vezzani (S3, CNR-Istituto di Nanoscienze)*

Superdiffusion is an interesting and complex phenomenon, observed in transport in highly heterogeneous random media, ranging from engineered experimental samples, to rocks and clouds. These disordered systems are typically composed of regions with very different diffusion properties, so that the transport process can be described as a Lévy walk: motion consists of a sequence of scatterings followed by long jumps in non scattering regions. Two concurrent effects make the problem particularly hard: the quenched randomness, inducing correlation between displacements, and, if the system is heterogeneous on all scales, the typical broad distribution of the steps length, which can be heavy tailed and Lévy distributed. While uncorrelated Lévy walks are well understood, the correlation effects, which are expected to exert a deep influence on the diffusion properties, are still to be characterized.

We consider correlated Lévy walks on a class of deterministic and random Lévy structures, modeled on recent experimental settings, with correlation between steps induced by their geometry. We characterize their superdiffusive behavior by a "single long-jump approximation" that estimate rare events effects, and by a scaling analysis, which applies to experimentally relevant quantities, such as mean square displacement and transmission probabilities.

**#401 - Field-induced superdiffusion and dynamical heterogeneities in one-dimensional models of glasses***Giacomo Gradenigo - Laboratoire Interdisciplinaire de Physique (LIPhy)*

*Other Authors: Giulio Biroli (CEA, Saclay), Eric Bertin (LIPhy, Grenoble)*

We show here that a probe particle immersed in a one-dimensional model of glass has a transient superdiffusive behaviour when pulled by an external field.

We explain how this anomalous transport property is related to dynamical heterogeneities, namely to the broad distribution of time-scales typical of a glass-former at low temperatures. Results of simulations are compared with exact results obtained by means of the Montroll-Weiss equation.

#### #402 - Non-isothermal Brownian motion

*Gianmaria Falasco - University of Leipzig*

*Other Authors: Klaus Kroy, Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, D-04009 Leipzig, Germany*

The theory of isothermal Brownian motion relies on fundamental principles of equilibrium classical statistical mechanics, such as the equipartition theorem, embedded in the stochastic framework of the Langevin equation. In the presence of a nonisothermal solvent it becomes questionable whether a Langevin-like description still applies and, if so, no general criterion exists which uniquely determines friction and thermal fluctuations. Starting from the fluctuating hydrodynamics of a solvent in local equilibrium, we constructively show that a generalized Langevin description does hold and derive the statistics of the corresponding thermal noise. The coupling between the hydrodynamic modes excited by the particle itself and the solvent temperature gradient turns the Langevin noise energy spectrum into a frequency-dependent tensor. We derive an explicit expression for this energy spectrum in the analytically tractable case of hot Brownian motion, i.e. a constantly heated particle generating a comoving radial temperature field. This allows us to explain the break of energy equipartition and express the energy content of the particle velocity and position in terms of effective temperatures.

#### #403 - cooperative and noise in excitonic quantum transport

*Fausto Borgonovi - dipartimento di matematica e fisica, università cattolica*

Natural photosynthetic systems interact with different environments, which are a source of noise but can also induce cooperative coherent effects, such as superabsorption of light and supertransfer of excitation. Both cooperativity and noise can be essential to achieve efficient energy transport in natural complexes and in bio-inspired quantum devices.

We show this point with the aid of the non Hermitian Hamiltonian approach to open quantum systems and analyzing both general quantum disordered networks and realistic models of photosynthetic antenna complexes (such as LHI, FMO).

**#404 - Adsorption properties of linear-cyclic polymer blends**

Giuseppe Pellicane (I) - University of Kwazulu-Natal

Other Authors: Mesfin Tsigie Department of Polymer Physics, University of Akron, Illinois, USA Mireille Megnidio-Tchoukouegno School of Chemistry and Physics, University of Kwazulu-Natal, Private Bag X01, Scottsville 3209, Pietermaritzburg, South Africa

We report a molecular dynamics study of bead-spring models of linear-cyclic polymer mixtures in the presence of vacuum interface. We focus on the regime of low cyclic polymer composition, and we show evidence that the density of linear polymers is enhanced with respect to the *bulk*, counter-intuitively as what is expected on the basis of recent theoretical predictions.

We analyze a number of interfacial properties versus their *bulk* counterparts, including the radius of gyration and the mobility of polymer chains. We also provide details about the percolation of the different polymer species.

**#405 - Liquids under electric fields: from water dissociation to Miller-like experiments**

A. Marco Saitta (I) - Université Pierre et Marie Curie - Sorbonne

Other Authors: Franz Saija (IPCF - CNR Messina), Giuseppe Cassone (Univ. Messina & UPMC Paris), Paolo V. Giaquinta (Univ. Messina), Fabio Pietrucci (UPMC Paris), François Guyot (UPMC Paris)

Since a few years, thanks to Berry-phase theory and its implementation in DFT schemes, it is possible to study the effect of finite homogenous electric fields in ab initio molecular dynamics simulations [1]. Here we present a study of bulk liquid water under intense electric fields [2]. We observe that the hydrogen-bond length and the molecular orientation are significantly modified at low-to-moderate field intensities. Fields beyond a threshold of about 0.35 V/Å able to dissociate molecules and sustain an ionic current via a series of correlated proton jumps, in good agreement with experimental values [3]. Upon applying even more intense fields ( $-1.0$  V/Å), a 15%-20% fraction of molecules are instantaneously dissociated and the resulting ionic flow yields a conductance of about  $7.8 \text{ } \Omega^{-1} \text{ cm}^{-1}$ . We then undertake the first ab initio computer simulations of the celebrated Miller experiment, that we perform in the condensed phase [4]. Our study shows that glycine spontaneously forms from mixtures of simple molecules once an electric field is switched on. Moreover, combining the electric field approach with a metadynamics-based analysis of chemical reactions [5], we identify formic acid and formamide as key intermediate products of the early steps of the Miller reactions, and the crucible of formation of complex biological molecules.

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**#406 - The role of convex polyhedra in supercooled water and ice nucleation**

Fausto Martelli (I) - Princeton University

Other Authors: Jeremy C. Palmer Huston University Pablo Debenedetti Princeton University Robert Car Princeton University

Combining the information on the first and the second shell of water, we introduce a new order parameter which directly links the degree of local order to the formation of convex polyhedra (1) classified in Euclidean geometry as Archimedean (2) and Johnson solids (3).

We apply our new order parameter to the case of supercooled ST2 water model at various thermodynamical conditions. The distribution of our order parameter turns out to be trimodal in the free energy landscape at the coexistence point (4), well separating high density liquid, low density liquid and cubic ice.

We observe that high density liquid doesn't show any ordered environment, while low density liquid possesses quasi well defined polyhedra topologies. Furthermore, nucleation turns out to be a process that does not involve the first coordination shell but only the second one, resulting in a competition amongst two frustrated polyhedra structures.

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**#407 - Phase portrait of a system near and above the threshold of thermodynamic stability**

Santi Prestipino - University of Messina and CNR-IPCF Messina

Other Authors: Gianpietro Malescio (University of Messina)

Stabilized dispersions of macromolecules are most easily described in terms of the effective interaction between the centers of mass of the molecules. For polymer chains, dendrimers, etc., the effective pair potential is *finite* at the origin, meaning that full overlap of the "particles" is allowed. Using a double-Gaussian model (DGM) for demonstration, we studied the system behavior as a function of the attraction strength  $\eta$ . According to a rigorous statistical-mechanical analysis, above a critical strength  $\eta_{c}$ , the infinite-size DGM system should eventually collapse to a finite cluster. As  $\eta_{c}$  is approached from below, we found that the liquid-vapor coexistence region widens substantially at low temperature, until the liquid density diverges right at  $\eta_{c}$ . Above the stability threshold, a well-definite boundary line (BL) divides the thermodynamic plane in two regions, differing in the value of the mean waiting time for collapse (being small on one side of the boundary, while much larger or even infinite in the other region). Upon adding a small hard core to the DGM potential, stability is recovered and the BL is converted to the spinodal line between two fluid phases. We find an interesting parallel between the destabilization of a colloidal dispersion, as induced by e.g. the addition of salt, and the process by which an increase in  $\eta$  brings eventually the state of a stabilized-DGM system inside the fluid-fluid spinodal region.

#### #408 - Cellulose degradation revealed by NMR spectroscopy

*Carmelo Corsaro - IPCF-CNR Messina*

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The understanding of deterioration pathways of cellulosic materials upon aging can be achieved by studying the hydration process and by identifying the products arising from cellulose degradation. In fact, the interaction with water molecules provokes modification of cellulose supermolecular structure and shifts the kinetic equilibrium of chemical reactions, such as acidic hydrolysis and oxidation, causing the formation of different by-products. The detailed knowledge of these processes is essential in improving conservation strategies and durability of cellulosic cultural heritage.

We use proton High-Resolution Magic Angle Spinning (HR-MAS) NMR spectroscopy in order to study the structural composition and dynamics of cellulosic samples as a function of the environmental humidity and samples' aging. In particular, we measure the proton relaxation times (both longitudinal and transverse) of the macroscopic magnetization to shed light on the interaction between cellulose and water. The used experimental technique is able to separate the contribution of the different types of water that can be found within cellulosic pores and fibers, by measuring the corresponding relaxation times. Furthermore, we detect different products of cellulose degradation in solid paper samples. For example, our results evidence the presence of simple and complex carboxylic acids. Since these products can catalyze further degradation, their knowledge is fundamental in order to plan conservation strategies of historical documents.

#### #409 - Recalescence from supercooled water

*Francesco Aliotta - CNR-Istituto per i Processi Chimico-Fisici*

*Other Authors: Paolo V. Giaquinta (Dipartimento di Fisica e di Scienze della Terra, Università di Messina), Rosina C. Ponterio (CNR-IPCF, Messina), Santi Prestipino (Dipartimento di Fisica e di Scienze della Terra, Università di Messina), Franz Saija (CNR-IPCF, Messina), Cirino Vasi (CNR-IPCF, Messina).*

A supercooled liquid returns, in a finite time, to stable thermodynamic equilibrium. The path towards equilibrium begins as a fast process which adiabatically drives the system to solid-liquid coexistence. Hence, the usual description of solid nucleation as an isothermal-isobaric process is inherently wrong because the phase transition can be isothermal only under coexistence conditions (1). Irrespective of the homogeneous or heterogeneous character of solid nucleation, the appearance of the first solid embryo causes the immediate release of latent heat to the liquid, unavoidably accompanied by large fluctuations of the local temperature. In this respect, it is clear that the escape from the metastable state towards the stable equilibrium condition, consisting of a solid/liquid mixture at the coexistence temperature, is an intrinsically non-equilibrium phenomenon and a complex process. At a mesoscopic level, this implies the occurrence of self-organization. The solidification never proceeds isotropically and the formation of dendrites is always observed. Dendrite formation is required for an efficient flow of latent heat by transport processes at the interface. In spite of these considerations, most current theories are limited to mathematical descriptions of branchless *needle crystals* growing steadily. Accurately describing the dendritic process is of paramount importance for understanding the thermodynamics of these irreversible processes. In this work, we report the results from an experimental investigation (through fast imaging and synchronous local temperature monitoring) of the dendritic growth in supercooled bulk water. Our experiments reveal that temperature reaches locally its coexistence value in a time of the order of few hundredths of a second (or shorter) when the supercooling temperature is lower than 266K, while a definitely slower evolution is observed for smaller undercooling. The transition between the two regimes takes place over an extremely narrow temperature range. The analysis of the results and their comparison with theoretical indications give some hints for a better understanding of this interesting and appealing phenomena.

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**#410 - Proton transfer in liquid methanol**

Giuseppe Cassone - Université Pierre et Marie Curie - Sorbonne Université

Other Authors: Paolo V. Giaquinta (University of Messina); Franz Saija (Institute for Chemical-Physical Processes of the Italian National Research Council - Messina); Antonino Marco Saitta (Université Pierre et Marie Curie - Sorbonne Université (Paris, France), and French National Centre for Scientific Research - CNRS).

Proton conduction in molecular liquids under an external or local electric field is a key phenomenon in many branches of science, from electrolysis to neurobiology but its microscopic description is difficult to achieve experimentally. In the last decade, thanks to Berry-phase theory and its implementation in density functional theory (DFT) schemes, it has been possible to study the effect of finite homogeneous electric fields in *ab initio* molecular dynamics simulations. Recently, relying on this approach, proton transfer in water has been studied with *ab initio* methods in bulk liquid water<sup>1</sup>. Here we report on a detailed systematic first-principles study of the effect of an external electric field in liquid methanol<sup>2</sup>. The results are compared with the water case. In particular, we observe that fields beyond a threshold value of about 0.30 V/Å are able to induce instantaneous molecular dissociations. By increasing the field intensity over 0.35 V/Å a sustained ionic current is measured as for the water. However, the resulting ionic conductivity ( $\sim 0.40 \text{ S cm}^{-1}$ ) is at least one order of magnitude lower than that of water, a circumstance that evidences a lower efficiency of proton transfer processes. We interpreted this difference by considering the field-induced fluctuations in the H-bond distribution of the ionic solvation shells.

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**#411 - Friction, phase changes and earthquake physics***Giulio Di Toro (I) - University of Manchester*

Earthquakes mostly originate on preexisting faults and occur because faults weaken with increasing slip and slip rate. It follows that frictional evolution of fault materials is of paramount importance in controlling the seismic rupture and slippage. Because of the large stresses (hundreds of MPa at >10 km depth) and slip rates (about 1 m/s) involved, a large amount of frictional work rate (product of frictional shear stress per slip rate) is dissipated along faults during earthquakes. The frictional work rate can be so large (1 to 100 MW m<sup>-2</sup>) as to grind and mill the rock (producing particles of nanometric size, or nanopowders), trigger mechanically and thermally activated chemical reactions, and, eventually, melt the rock. Under these extreme deformation conditions, the fault surfaces are separated by fluids or other tribochemical products (melts, gels, nano-powders, amorphous, dehydration and decarbonation products, etc.). It follows that earthquake physics is controlled by the mineral reactions and phase changes triggered by the passage of the seismic rupture and, as a consequence, by the rheology of the reaction products. Here, by exploiting the results of (1) field and microanalytical studies conducted on natural fault products, and (2) experimental studies reproducing the extreme deformation conditions typical of seismic slip, we will discuss the mineral reactions and phase changes concomitant to and responsible of fault weakening during earthquakes.

**#412 - Monitoring Volcanoes at Global Scale by Acoustic waves***Maurizio Ripepe (I) - University of Florence**Other Authors: Emanuele Marchetti (University of Florence), Giorgio Lacanna (University of Florence), Giacomo Olivieri (University of Florence)*

Volcanoes are quite a prolific radiator of acoustic waves. Gas rapidly expanding in the conduit produce infrasound providing insights into eruption dynamics. Linear theory of sound explains acoustic pressure in terms of outflow mass rate and this has strong implications for explosive dynamics. Large explosive volcanic eruptions typically generate a plume of hot ash and debris ejected into the atmosphere and inducing pressure perturbation with frequency content ranging from 0.1-4 Hz down to 1-2 mHz typical of gravity waves. These waves can be recorded thousands of kilometers away by distant stations. Our ability to detect these pressure waves can be used to track the ash plume evolution providing the time history of the excess pressure and reflecting the explosive gas emission. This information could be used as input parameter in the simulations of the ash cloud dispersal in the atmosphere contributing to a correct risk assessment for civil aviation. Infrasound can be generated also by non-explosive linear sources such as pyroclastic flows, providing crucial information to volcano monitoring and risk management. Volcano acoustics integrated with other geophysical measurements, particularly seismic, thermal and ground deformation may assist with their interpretation leading to important understanding of the volcano dynamics and substantially improving the forecast of volcano-related hazards.

**#413 - Measurements of ground deformations and their interpretation***Giuseppe Puglisi (I) - Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Catania - Osservatorio Etno*

Thanks to the rapid evolution of the geodetic techniques during the last decades, the ground deformation monitoring has become a key approach to investigate about the dynamics of active areas (e.g.; volcanoes, seismic faults). Currently we are able to cover the whole spectrum of deformations, both on time and space domains, allowing to investigate crustal geodynamic processes that originate at different depths and affect areas large up to several hundreds of kilometers. The availability of so large amount of data coupled with the continuous improvements on the computing resources stimulated the implementation of new approaches for the data analysis.

The information contained in the deformation data sets is thus exploited to find anomalies in the signals or to fix the parameters of physical models underlying geodynamic processes such as volcanic eruptions or earthquakes.

The talk will give an overview of the current advanced ground deformation monitoring techniques and data analysis methods by presenting some recent case studies.

**#414 - An observatory for rotational seismology in the underground Gran Sasso National Laboratory***Nicolò Beverini - Università di Pisa**Other Authors: J. Belfi, A. Di Virgilio (INFN, sezione di Pisa); A. Ortolan (INFN, Lab. Naz. di Legnaro); A. Porzio (CNR, SPIN, Napoli); G. De Luca, G. Saccorotti, (INGV); R. Santagata (Università di Siena)*

The lack of instrumentation with suitable sensitivity has prevented up to the recent years the observation of the ground rotations induced by the seism, although the relevance of this knowledge was well recognize in the literature. The development of large ring laser gyroscopes (RLG), based on the Sagnac effect and equipped with state-of-art high reflective mirrors, made possible to open this new field of study, involving many areas of geophysics, from geodesy to seismology to the monitoring of critical structures.

Nowadays the G-ring apparatus in Wettzell (Germany) represents the reference RLG for geodetic and seismological observations. It is a square laser cavity with 4 m of side around a monolithic bloc of Zerodur, (a glass with null thermal dilation factor), with a record sensitivity of 10<sup>-13</sup> rad/s, allowing important results from geodesy spanning to the analysis of earthquakes at tele-seismic distances.

A similar apparatus, much less expensive, has been mounted in the tunnel of the INFN Gran Sasso National Laboratory as a first step of a larger project of fundamental physics aiming to detect very thin General Relativity effect on the Earth rotation rate. It consists in a large He:Ne ring laser with a 3.6 meters side square cavity installed over a granite structure integral to the rock in the B knot tunnel. In the first experimental runs we observed a sensitivity better than  $10^{10}$  rad/s, which make it suitable to observe rotational seismic noise in the 1000 s - 50 Hz bandwidth. The deep underground location will effectively isolate the instrument from meteorologic and anthropic noise.

To fully exploit the seismic detection potentiality, in the box with the RLG we have installed auxiliary instrumentation constituted:

- A Nanometrics Trillium 360s seismometer, which is also part of the national earthquake monitoring program of the INGV. It will provide the data to be compared to the RLG's rotational data in order to infer a phase velocity measurements during the transit of shear waves from earthquakes.
- A second more performing broadband seismometer (Guralp CMG 3T-360s) in order to obtain better estimates of differential velocities and for data redundancy.
- A Lipmann 2-K digital tilt-meter with a resolution better than 1 nrad, placed beside the seismometer in order to monitor the possible slow ground tilt related to either local or wide scale (solid earth tides) effects.

The preliminary results on seismic data analysis will be presented.

#### #415 - Mechanical origin of aftershocks

*Eugenio Lippiello - Department of Mathematics and Physics Second University of Naples*

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Aftershocks are the most striking evidence of earthquake interactions and the physical mechanisms at the origin of their occurrence are still intensively debated.

Novel insights stem from

recent results showing that aftershock occurrence in time and magnitude is controlled by the faulting style.

Our study shows that the size of the aftershock zone is a measure of the level of differential stress.

We find that positive correlations among parameters controlling aftershock organization in time, energy and space are a stable feature of seismicity independently of magnitude range and geographic areas.

We explain the ensemble of experimental findings by means of a description of the Earth Crust as an heterogeneous elastic medium coupled with a Maxwell viscoelastic asthenosphere.

Our results show that heterogeneous stress distribution in an elastic layer combined with a coupling to a viscous flow are sufficient ingredients to describe the physics of aftershock triggering.

#### #416 - Towards the numerical modelling of volcano aeroacoustic source processes using Lattice Boltzmann strategies

*Federico Brogi - University of Geneva*

*Other Authors: C. Bonadonna\*, O. Malaspina\*, M. Ripepe\*\*, B. Chopard\*, J. Latt\*, J. Falcone\* \* University of Geneva, Switzerland; \*\* University of Florence, Italy.*

Low frequency (<20Hz) acoustic measurements have a great potential for the real time characterization of volcanic plume source parameters. Nonetheless many shortcomings have been highlighted in the understanding of the acoustic monitoring. In particular, the application of the classical acoustic source models to volcanic explosive eruptions has shown to be challenging and a better knowledge of the link between the acoustic radiation and actual volcanic fluid dynamics processes is required. New insights into this subject could be given by the study of realistic aeroacoustic numerical simulations of a volcanic jet. Lattice Boltzmann strategies (LB) provide the opportunity to develop an accurate, computationally fast, 3D physical model for a volcanic jet and wave propagation. In the field of aeroacoustic applications, dedicated LB schemes has been proven to have the low dissipative properties needed for capturing the weak acoustic pressure fluctuations. However, when dealing with simulations of realistic flows, artificial boundaries are defined around the flow region. The reflected waves from these boundaries can have significant influence on the flow field and overwhelm the acoustic field of interest. A special absorbing boundary layer has been implemented in our model to suppress the reflected waves. In addition, for highly multi-scale turbulent flows, such as volcanic plumes, the number of grid points needed to represent the smallest scales might become intractable and the most complicated physics happen only in small portions of the computational domain. The implementation of the grid refinement, in our model allow us to insert local finer grids only where is actually needed and to increase the size of the computational domain for running more realistic simulations. 3D LB model simulations for simple benchmark problems as well as for the more complex jet aeroacoustics have been accurately validated. Both mean flow and acoustic results are in good agreement with theory and experimental data available in literature.

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**#417 - Elicitation Experiment at Etna Volcano**

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Advances in volcano monitoring and forecasting need a multidisciplinary collaborative framework. In light of this, a Bayesian Event Tree (BET) approach was performed, whose central element is the interpretation of probability distributions of events as a conditional measure of uncertainty (on a [0, 1] scale) about the occurrence of the same in specific conditions.

The definition of what is background vs anomaly represents the core of the analysis, i.e., the selection of geophysical, volcanological and geochemical parameters and the quantitative definition of anomalies.

At Mt. Etna different pre-eruptive observations, with different timescales (from months to days/hours), are recorded. A subjectivity is often the feeling expression of an incoming event, and to minimize such a sensation, an expert opinion can be used.

Weighting of experts varies, even though equal-weighted procedures are still considered. For the present analysis, a consensus-based expert scoring scheme and an expert elicitation method are adopted. In this process, expert opinion is weighted on the basis of mutual recognition among experts expressed through a regularly repeated blind procedure.

In detail, for each node of the BET, for each parameter (using scores and votes; in this latter case, all the experts have weight equal to 1) average, median, and 10<sup>th</sup> and 90<sup>th</sup> percentiles of the selected thresholds are estimated. A different setting regards the thresholds aimed to accept the selected parameters, being evaluated by considering marked slope changes, if they occur in scores and votes plots.

The INGV, both Osservatorio Etneo (Catania) and Palermo Section, experienced Elicitation I, which involved 40 (out of 58; ca. 70%) experts who selected parameters and relative critical thresholds at each node of the ET.

Regarding to the scores analysis (weights obtained from scores), it is roughly equivalent to votes analysis for nodes 1 (Unrest) and 2 (Unrest Cause), while significant differences appear at node 3 (Eruption). In particular, both at nodes 1 and 2 there seems to be a single parameter that has been selected by the majority of experts (among them, some of those with higher score), while all the other proposed parameters do not aggregate a large consensus and are selected by minorities. At node 3, it appears that the highest score's experts have voted a few unpopular parameters, while the most popular ones have a low total score (meaning that the low score's parameter have selected it).

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**#418 - Nonlinear x-ray wave mixing**

Sharon Shwartz (I) - Bar Ilan University

Today, nonlinear optics is primarily focused on the infrared to the visible regimes. In this spectral range, concepts and techniques based on nonlinear optics are implemented in many diverse fields. For example, laser technology, optical communication, ultrafast science, quantum optics, and nonlinear spectroscopy techniques. The high brightness and peak power of the new x-ray free-electron lasers has opened the possibilities of performing novel experiments in the field of nonlinear optics at very short wavelengths, and of extending concepts from the optical regime into the x-ray regime. X-ray nonlinearities are very different from conventional nonlinearities in the optical regime, thus their study is interesting in its own right and may lead to new important applications.

I will describe recently performed experiments demonstrating nonlinear x-ray wave-mixing including x-ray and visible wave mixing, x-ray second harmonic generation, and x-ray parametric down-conversion. I will present theoretical studies of difference-frequency generation of optical radiation from two-color x-ray pulses, and x-ray-pulse characterization by spectral shearing interferometry. I will discuss future directions of exploring nonlinear and quantum effects in the x-ray regime. For example, x-ray parametric down-conversion may be developed into a very powerful method to study fundamental effects in quantum optics. X-ray and visible mixing may lead to atomic scale resolution techniques to study chemical bonds. Nonlinear techniques are expected to be useful in the inspection of sub-femtosecond temporal pulses.

**#419 - Nonlinear pump-probe spectroscopy for x-ray free-electron laser applications**

Victor Kimberg (I) - Department of Theoretical Chemistry and Biology, Royal Institute of Technology

Recent invention of the x-ray free electron laser (XFEL) opens new possibilities in pump-probe spectroscopic schemes extended to x-ray energy range. First, use of x rays addressing deep core-electrons makes x-ray spectroscopy extremely element and site selective. Second, short (femtosecond) XFEL pulse duration is comparable to a typical scale of nuclear dynamics in molecules, as well as to charge or excitation transfer in complex compounds, allowing to resolve the ultra-fast processes in the pump-probe experiment. Finally, high intensities available from XFELs allow to trigger stimulated emission and to study nonlinear effects in the x-ray energy range. Combination of the all above features in the XFEL based pump-probe techniques provide unique framework for many new applications in atomic and molecular physics, biology and material science.

In the present talk I would like to overview our recent theoretical results on pump-probe spectroscopy using short intense x-ray and optical pulses. I will start by presenting principles of IR-x-ray phase sensitive pump-probe spectroscopy and discuss its possible applications [1]. Then I will focus on all x-ray pump-probe schemes including stimulated emission and lasing [2], stimulated resonant inelastic x-ray scattering [3], and resonant Auger scattering as control tools for wave packet dynamics in molecular systems. I will also address experimental feasibility for high-resolution nonlinear pump-probe and stimulated x-ray Raman spectroscopies. I will conclude by discussing recent experimental results on nonlinear x-ray pump-probe studies at LCLS motivated by our theoretical predictions.

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**#420 - Extreme ultra violet four wave mixing experiments: from table top lasers to fourth generation light sources**

Riccardo Cucini (I) - Elettra-Sincrotrone Trieste

Other Authors: Andrea Battistoni (Stanford University), Filippo Bencivenga (Elettra-Sincrotrone Trieste), Claudio Masciovecchio (Elettra-Sincrotrone Trieste)

The current construction of the FERMI@Elettra Free Electron Laser (FEL) facility will make available Vacuum Ultra Violet (VUV) photon pulses with unique characteristics [1]. The peculiarities of this source will be exploited in order to develop a time resolved instrument (TIMER) based on the transient grating scheme. TIMER would be able to probe the collective atomic dynamics in a momentum ( $Q=0.02\div 1.2\text{ nm}^{-1}$ ) and energy transfer ( $E=0.1\div 10000\text{ }\mu\text{eV}$ ) region that, to date, cannot be accessed by any time or energy resolved instrument [2].

Particularly, the Q-range exploitable by TIMER is of special interest for the study of disordered systems, since it corresponds to the characteristic length scale ( $\sim 10\div 100\text{ nm}$ ) of topological disorder. On such length scale the dynamical behavior of amorphous solids

still presents unsolved and strongly debated. Though the study of collective dynamics at the nanoscale is of the greatest relevance in order to understand the phenomenology of the glassy phase, it is actually hampered by the technical impossibility to experimentally probe the 0.1-1 nm<sup>-1</sup> Q-range. This harsh limit would be overcome by TIMER. The unique capabilities of TIMER would also provide a sensitive probing of interfaces and thin films, as well as heat transport and electron correlations in nanostructured materials. Different Four wave mixing setups are presented, based on sources ranging from infrared to the extreme ultraviolet region. Each scheme introduces variations with respect to the previous one, allowing moving from classical table top laser experiments towards a new four wave mixing scheme based on free electron laser radiation. A comparison between the various setups, the first results from extreme ultra violet transient grating experiments [3], and the actual state of the new beamline will be discussed.

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#### #421 - Coherent control in the extreme ultraviolet spectral range using the Free Electron Laser FERMI@Elettra

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Coherent control with lasers involves steering a quantum system along two or more pathways to the same final state, and manipulation of the phase and wavelength of light to favour this state. In some cases this is an interference effect between transition matrix elements, e.g.  $M_{\{1\}}e^{i\varphi_{\{1\}}}$ , and  $M_{\{2\}}e^{i\varphi_{\{2\}}}$ , where the relative phase  $\Delta\varphi = \left(\varphi_{\{2\}} - \varphi_{\{1\}}\right)$  between the two paths makes it possible to manipulate the final outcome.

Coherent control has already been demonstrated in the visible domain, where coherent light pulses with different wavelengths can be generated by nonlinear crystals and the relative phase can be controlled by delaying one pulse with respect to the other. In the XUV spectral range, however, this approach poses severe challenges due to the lack of suitable delay lines for the control of the relative phase between different spectral components.

In this work we demonstrate for the first time coherent control in the XUV domain by exploiting the unique characteristics of the seeded FEL FERMI@Elettra. In the experiment two harmonic fields, a fundamental  $\omega$  and its second harmonic  $2\omega$ , were generated by the same electron bunch in the first five and the last undulator of FERMI, respectively. An electron delay line between the fifth and sixth undulators was introduced to slightly delay the arrival of the electron bunch in the second section, thus resulting in a phase delay between the  $\omega$  and  $2\omega$  components.

Neon atoms were irradiated by the combination of the two harmonic fields. The fundamental was tuned at the photon energy  $\hbar\omega = 19.68\text{eV}$  corresponding to the excitation of the 4s level. The two-photon path corresponds to photoionization with an outgoing p-wave through the 4s-resonance, while the single-photon path causes the ejection of an s- or d-wave electron directly from the 2p orbital. The interference of the linear and nonlinear paths leads to an asymmetric photoelectron angular distribution that can be quantified in the left-right asymmetry parameter  $A_{\{LR\}} = \left(N_{\{L\}} - N_{\{R\}}\right) / \left(N_{\{L\}} + N_{\{R\}}\right)$ , where  $N_{\{L\}}$  and  $N_{\{R\}}$  indicate the number of photoelectrons emitted to the left and right, respectively.

This asymmetry was measured as a function of the relative phase between the two fields. Phase differences corresponding to a delay of 10 attoseconds were introduced. A clear modulation (depth of 12%) was observed, indicating the effective control of the emission direction of the photoelectron wave packet.

Corresponding numerical calculations, performed by either solving the time-dependent Schrödinger equation directly on a space-time grid in a single-active electron model or by applying second-order nonstationary perturbation theory, support the experimental findings.

#### #422 - Observing sub-nanosecond strain dynamics in a GeTe/Sb2Te3 crystalline superlattice by means of resonant time resolved x-ray absorption spectroscopy

Marco Malvestuto - Elettra-Sincrotrone Trieste

Other Authors: Barbara Casarin (Elettra-Sincrotrone Trieste), Antonio Caretta (Elettra-Sincrotrone Trieste), Fulvio Parmigiani (University of Trieste)

Here we use ultrafast optical pump pulses to induce dynamical strain and stroboscopically measure the corresponding lattice distortions in a GeTe/Sb2Te3 crystalline superlattice (CSL) using 100-ps x-ray pulses from the Elettra storage ring. An ab-initio strain model accounts for a good representation of the observed changes in the absorption signal. The information on the laser

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induced structural strains during the excitation process can lead to paramount insights into the mechanisms at the origin of the phase-change properties of CSL.

### #423 - Optical Gain from Polyfluorene Keto Defects in a Liquid Crystal Mixture

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In this work we show, by means of confocal photoluminescence measurements and fs pump-probe spectroscopy, that a large polarized stimulated emission from polyfluorene keto defects is obtained in a mixture of polyfluorene with a nematic low molecular weight Liquid Crystal (LC). This mixture is placed in 9-micron thick cell constituted by two polyamide-coated plates rubbed to induce a macroscopic optical anisotropy of the LC molecules. In this blend a peculiar phase separation generates an ordered network of LC-rich micro-domains with the most of the polyfluorene chains placed on the microdomains boundaries. These well-defined phase boundaries have an anchoring effect so strong that the polymeric chains are forced to align parallel to them, despite the alignment of the nematic LC induced by the rubbing layers. The isolation and orientation of the polymeric chains reveal the possibility to obtain polarized optical gain from the keto defect. The results are expected to have broad implications in the fields of photophysics and material design of polyfluorene materials, since the formation of few fluorenone units can be seen not anymore as a form of degradation of the polyfluorene but as an improvement of the physical properties of this interesting polymer.

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**#424 - Nonequilibrium fluctuations in quantum heat engines: Theory, example, and possible solid state experiments**

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*Other Authors: Rosario Fazio (NEST, Scuola Normale Superiore & Istituto Nanoscienze-CNR, I-56126 Pisa, Italy), Jukka Pekola (Low Temperature Laboratory, O.V. Lounasmaa Laboratory, Aalto University, FI-00076 Aalto, Finland)*

We study the stochastic energetic exchanges in quantum heat engines. Due to microreversibility, these obey a fluctuation relation, called the heat engine fluctuation relation, which implies the Carnot bound: no machine can have an efficiency larger than Carnot's efficiency. The stochastic thermodynamics of a quantum heat engine (including the joint statistics of heat and work and the statistics of efficiency) is illustrated by means of an optimal two-qubit heat engine, where each qubit is coupled to a thermal bath and a two-qubit gate determines energy exchanges between the two qubits. We discuss possible solid state implementations with Cooper pair boxes and flux qubits, quantum gate operations, and fast calorimetric on-chip measurements of single stochastic events.

**#425 - Total correlations of the diagonal ensemble herald the many-body localization transition**

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The intriguing phenomenon of many-body localization (MBL) has attracted significant interest recently, but a complete characterization is still lacking. In this work we introduce the total correlations, a concept from quantum information theory capturing multi-partite correlations, to the study of this phenomenon. We demonstrate that the total correlations of the diagonal ensemble provides a meaningful diagnostic tool to pin-down, probe, and better understand the MBL transition and ergodicity breaking in quantum systems. In particular, we show that the total correlations has sub-linear dependence on the system size in delocalized, ergodic phases, whereas we find that it scales extensively in the localized phase developing a pronounced peak at the transition. We exemplify the power of our approach by means of an exact diagonalization study of a Heisenberg spin chain in a disordered field.

**#426 - Phase-coherent thermal devices based on Josephson quantum nanocircuits**

*Francesco Giazotto (I) - NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore*

The Josephson effect represents perhaps the prototype of macroscopic phase coherence and is at the basis of the most widespread interferometer, i.e., the superconducting quantum interference device (SQUID). Yet, in analogy to electric interference, Maki and Griffin predicted in 1965 that thermal current flowing through a temperature-biased Josephson tunnel junction is a stationary periodic function of the quantum phase difference between the superconductors. In this scenario, a temperature-biased SQUID would allow heat currents to interfere thus implementing the *thermal* version of the electric Josephson interferometer.

In this presentation I shall initially report the first experimental realization of a *heat interferometer*. We investigate heat exchange between two normal metal electrodes kept at different temperatures and tunnel-coupled to each other through a thermal *'modulator'* in the form of a DC-SQUID. Heat transport in the system is found to be phase dependent, in agreement with the original prediction. Next, after introducing some basic concepts about diffraction of heat currents I shall present experimental results on the first quantum *'diffractor'* for thermal flux. Specifically, thermal diffraction manifests itself with a peculiar modulation of the electron temperature in a small metallic electrode nearby-contacted to a Josephson junction when sweeping the magnetic flux  $\Phi$ . The observed temperature dependence exhibits a clear reminiscence with a Fraunhofer-like modulation pattern, as expected fingerprint for a quantum diffraction phenomenon. Our results confirm a recent prediction of quantum heat transport and exemplify the complementary proof of the existence of phase-dependent thermal currents in Josephson-coupled superconductors.

Finally, I shall introduce the physics at the basis of thermal rectification with superconducting tunnel junctions, and show the first realization of an ultra-efficient low-temperature hybrid *'heat current rectifier'*, thermal counterpart of the well-known electric diode. Our design is based on a tunnel junction between two different elements: a normal metal and a superconducting island. Electronic heat current asymmetry in the structure arises from large mismatch between the thermal properties of these two. We demonstrate temperature differences exceeding 60 mK between the forward and reverse thermal bias configurations. This structure offers a remarkably large heat rectification ratio up to about 140 and allows its prompt implementation in true solid-state thermal nanocircuits and general-purpose electronic applications requiring energy harvesting or thermal management and isolation at the nanoscale. Our approach combined with well-known methods for phase-biasing superconducting circuits provides with a novel tool for mastering heat fluxes at the nanoscale.

**#427 - 3D-Quantum Integrated Optical Simulation***Fabio Sciarrino (I) - Sapienza Università di Roma*

Integrated photonic circuits have a strong potential to perform quantum information processing. Indeed, the ability to manipulate quantum states of light by integrated devices may open new perspectives both for fundamental tests of quantum mechanics and for novel technological applications. Within this framework we have developed a directional coupler, fabricated by femtosecond laser waveguide writing, acting as an integrated beam splitter able to support polarization-encoded qubits [1]. As following step we addressed the implementation of quantum walk. For the first time, we investigated how the particle statistics, either bosonic or fermionic, influences a two-particle discrete quantum walk [2]. As following step we have exploited this technology to simulate the evolution for disordered quantum systems observing how the particle statistics influences Anderson localization [3]. Finally we will discuss the perspectives of optical quantum simulation: the implementation of the boson sampling to demonstrate the computational capability of quantum systems and the development of integrated architecture with three-dimensional geometries [4]. We report the experimental observation of three-photon interference in an integrated three-port directional coupler realized by ultrafast laser writing. By exploiting the capability of this technique to produce three-dimensional structures, we realized and tested in the quantum regime a three-port beam splitter, namely a tritter, which allowed us to observe bosonic coalescence of three photons [5]. These results open new important perspectives in many areas of quantum information, such as fundamental tests of quantum mechanics with increasing number of photons, quantum state engineering and quantum simulation.

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**#428 - Landauer's principle in multipartite open quantum system dynamics***Salvatore Lorenzo - Dipartimento di Fisica e Chimica, Università degli Studi di Palermo*

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We investigate the link between information and thermodynamics embodied by Landauer's principle in the open dynamics of a multipartite quantum system. Such irreversible dynamics is modelled in terms of a collisional model with a finite temperature reservoir. We demonstrate that Landauer's principle holds, for such an open configuration, in a form that involves the flow of heat dissipated into the environment and the rate of change of the entropy of the system. Quite remarkably, such a principle for heat and entropy power can be explicitly linked to the rate of creation of correlations among the elements of the multipartite system and, in turn, the non-Markovian nature of their reduced evolution. Such features are illustrated in two paradigmatic cases.

**#429 - NEGATIVE ABSOLUTE TEMPERATURES VINDICATED***Pierfrancesco Buonsante - INO-CNR and QSTAR Center*

*Other Authors: Roberto Franzosi, INO-CNR and QSTAR Firenze Augusto Smerzi, INO-CNR and QSTAR Firenze*

Negative absolute temperatures emerge naturally from Boltzmann's definition of "surface" microcanonical entropy in isolated systems with a bounded energy density. Recently, the well-posedness of negative absolute temperatures has been challenged, on account that only Gibbs "volume" entropy—and the strictly positive temperature thereof—would give rise to a consistent thermodynamics.

Here we focus on a discrete nonlinear model characterized by bounded energy densities, describing the propagation of light in arrays of coupled waveguides. We present analytical and numerical evidence that Boltzmann microcanonical entropy provides a consistent thermometry for both signs of the temperature. In particular, we show that Boltzmann (negative) temperature allows the description of phase transitions occurring at high energy densities, at variance with Gibbs temperature. Our results are relevant also to ultracold gases trapped in optical lattices.

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**#430 - Nonclassical features in the distribution of work performed on a quantum system**

*Paolo Solinas - Istituto SPIN-CNR*

*Other Authors: Simone Gasparinetti, Department of Physics, ETH Zurich, Zurich, Switzerland*

The study of the statistics of work done on a driven quantum system is particularly tricky because of issues related to the measuring process. In the most used protocol, the system is measured at beginning and at the end of the evolution. In special cases in which the system is in a statistical mixture of energy eigenstates, this procedure alongside with a statistical sampling allows to reconstruct the work statistics. However, the first measure causes a wave function collapse and inevitably leads to a change in the system dynamics. Therefore, the protocol cannot be used if the system is initially in a generic initial state.

Here, we propose a novel approach to define and measure the statistics of work, internal energy and dissipated heat in a driven quantum system. In our framework the presence of a physical detector arises naturally and work and its statistics can be investigated in the most general case. In particular, we explicitly show that the quantum coherence of the initial state can lead to measurable effects on the moments of the work done on the system. At the same time, we recover the known results if the initial state is a statistical mixture of energy eigenstates. Our method can also be applied to measure the dissipated heat in an open quantum system. By sequentially coupling the system to a detector, we can track the energy dissipated in the environment while accessing only the system degrees of freedom.

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**#431 - Porphyrin molecules at interfaces**

Willi Auwärter (I) - Technische Universität München

Porphyrins and related tetrapyrrole molecules possess an impressive variety of functional properties - including axial ligation, electron transfer, light harvesting and catalytic transformations - that have been exploited in natural and artificial systems. From a surface science perspective, porphyrins are thus ideally suited as building blocks for surface-anchored functional nanostructures [1-3]. After briefly reviewing recent scanning tunneling microscopy and spectroscopy results addressing key aspects of such tetrapyrrole units with sub-molecular resolution, we will focus on two approaches yielding surface-anchored porphyrin systems with new properties. The first one bases on on-surface dehydrogenation and ring-closing reactions yielding novel porphyrinoids on Ag(111), including planar species [4], covalently linked dimers and longer oligomers [5]. We will discuss the impact of molecular symmetry on the reaction products and characterize them by high-resolution atomic force microscopy and complementary computational modeling based on density functional theory. In a second approach we use atomically thin boron nitride (BN) layers grown on Cu(111) as templates dictating the electronic level alignment of the porphyrin nanostructures [6] and supporting distinct coordination motifs of functionalized porphyrins upon exposure to metal adatoms [7]. In combination with the in-situ metalation of free-base porphyrins, mixed valence metal-coordination networks can be achieved on the insulating BN spacer layer. These approaches provide access to new porphyrin-based systems, complex metallo-supramolecular arrays and hybrid architectures with prospects for functionalities, e.g., in spintronics, photonics, or heterogeneous catalysis.

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**#432 - Metalation of porphyrins and the role of the interaction with surfaces**

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Metallo-porphyrin are a very important class of organic molecules for their possible use in novel organic devices based on the interaction of an active nanoscale site with the surrounding medium. Moreover, they can be taken as templates for the ordered organization of "isolated" metallic atoms, which correspond the metallic ions at the center of the macrocycles. The fine control on the self-assembling and, possibly, on the metalation of the molecules represent a key issues in the development of these organic-substrate interfaces with the aim of tailoring suitable properties for organic-based devices. Therefore it is fundamental to understand how porphyrins (metalated or not) interact with the substrates and in which way the self-assembled organic monolayer can be controlled and modified. Here we show several methods to metalate the metal-free porphyrins on surfaces, the modification of these molecules with temperature and the interaction of porphyrins with the substrate. In particular, we illustrate an interesting way to metalate the porphyrins by picking-up substrate metal atoms on the surface and how the surface oxidation can dramatically influence this process.

**#433 - On-surface synthesis of metal complexes, organic molecules and organometallic compounds**

J. Michael Gottfried (I) - University of Marburg

On-surface synthesis of metal complexes, organic molecules and organometallic compounds is a promising approach for surface modification and functionalization. Surface reactions in ultrahigh vacuum can produce compounds which are not accessible by conventional synthesis in solution or which are too large or too reactive for vapor deposition. Catalytic and template effects exerted by the surface can help driving the reaction into the desired direction. The first part of this contribution focuses on the surface-confined synthesis of large metal complexes based on porphyrins and phthalocyanines [1]. Monolayers and multilayers of these complexes are synthesized by reaction of the metal-free macrocycle ligands with coadsorbed metal atoms (or metal atoms from the substrate), sometimes followed by the attachment of another ligand on the metal center. Mechanistic details of this *in situ* redox reaction and properties of the resulting complexes will be discussed [1]. The second part deals with supramolecular

assembly and reactions of aryl bromides on metal surfaces. Temperature-dependent studies on Cu(111) show that the C-Br bonds dissociate already at low temperatures and are replaced by C-Cu-C bonds, which lead to the formation of linear, cyclic or two-dimensional organometallic oligomers and polymers. A prominent example for a molecule for which no solution-based synthesis is available, but which can be made by on-surface synthesis, is hyperbenzene, a hexagonal octadecaphenylene, which is formed by an Ullmann type reaction from six dibromo-*m*-terphenyl molecules [2]. As a room-temperature stable intermediate, the corresponding organometallic macrocycle with 6 C-Cu-C bridges was found, accompanied by other cyclic and chain-like organometallic oligomers [3]. On Ag(111), the intact aryl bromides form supramolecular structures linked by halogen bonds, for example fractals with the topology of Sierpinski triangles [4].

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#### #434 - Exploring the structural and electronic properties of Graphene on intercalated magnetic layers: an experimental and theoretical study

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Investigating Graphene (Gr) structural, electronic and magnetic properties has been the main focus of surface science in the last decade. On the one hand, a fascinating perspective was represented by the possibility of observing the exotic effects predicted for this novel material, as the Dirac fermion like dispersion for the low energy charge carriers. On the other hand, many efforts have been devoted to tune Gr properties, aiming at implementing state-of-the-art technological devices with Gr-based components. To obtain the desired tuning, a rewarding approach is to exploit Gr mutual interaction with its environment, as supporting metallic buffer layers and adsorbates. The electronic, structural and magnetic properties of Gr have been proved to be very susceptible to such interaction and, to date, many different configurations have been achieved: free-standing like Gr can be grown exploiting weak physisorption on Ir(111), along with a gentle and regular corrugation; an enhanced and still regular corrugation can be achieved on Ru(0001); a magnetic anisotropy can be induced by coupling the carbon sheet with a magnetic substrate like Ni(111).

We present our results on the intercalation of a monolayer of Co atoms underneath a pristine Gr crystal grown on Ir(111). The intercalation of a metallic species different from the initial buffer-layer one is a suitable approach to obtain new hybrid configurations. In particular we focused on: the intercalation dynamics and the structural transition induced by the Co interstitial layer, as probed by fast X-ray photoemission spectroscopy (XPS); modification of the valence and conduction band electronic configuration, by means of angle resolved photoemission spectroscopy (ARPES) and near edge absorption fine structure (NEXAFS) spectroscopy. Further insight in our experimental results is provided by density functional theory calculations. The aim of the calculations is to shed light on the C-Co hybridization process, in order understand the experimentally observed modification in the valence and conduction density of states.

#### #435 - Modeling Organic thin film transistors: a journey from electronic to biological applications.

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Organic Thin Film Transistors (OTFT) are metal-insulator-semiconductor field-effect transistors in which the semiconductor is a conjugated organic material. Such devices have a wide range of applications requiring multi-layer layouts with a various degree of complexity. Herein, we face the challenge of understanding their functioning at an atomistic scale by means of different computational techniques, ranging from quantum mechanics (QM) calculations to classical Molecular Dynamics (MD) simulations. In particular, we focused our attention on two widely used semiconductor polymers, P3HT and PBTBT [1]. Our results describe how their different morphology and order influence the charge transport properties in the crystal and the amorphous phases [2]. The combined application of MD and periodic Density Functional Theory unveils that the morphology of the semiconductor layer and the hole mobility are strongly affected by the self assembled monolayer employed as a substrate [3].

The application of a combined experimental/theoretical approach allowed us also to assess how functionalized OTFTs can be used as a microscopic laboratory that is able to reveal protein functioning upon binding small organic compounds [4-5], as, for instance,



in the employment of OTFTs in the construction of an electronic nose that would be able to detect molecules of biological as well as environmental interest.

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#### #436 - Supramolecular engineering of 2D molecular arrays: porphyrins conformation and metalation on metallic substrates

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Porphyrins are used to fabricate 2D arrays, where metallic centers with nanometer spacing can be inserted. Tailoring the interfacial properties of such templates at the surface of metals or semiconductors, constitutes a basic step towards the exploitation of heterogeneous tools, like magnetic, catalytic or opto-electronic devices. free base molecules or directly uptaken from the suitable substrate. The number of very recent publications on the subject testify that the porphyrin-metal interaction represents an hot topic in the field of chemistry and physics of materials [1,2].

We have shown that an annealing at ~550 K of 2H-TPP (tetraphenyl porphyrin) monolayer templates on Ag(111), triggers the irreversible rotation of the phenyl rings into a coplanar molecular structure, while the room temperature adsorbed 2H-TPP monolayers should have phenyl rings tilted by ~30-60° with respect to the macrocycle that is typically parallel to the surface plane [3,4]. By means of polarization dependent near edge X-ray absorption spectroscopy (NEXAFS) it is possible to directly probe the rotation of the phenyl rings upon surface annealing. Having established the methodology for a direct evaluation of the molecule-substrate interaction, by means of a combination of X-ray absorption and photoemission spectroscopies, here we focus on the role of the metal core in the porphyrin macrocycle with respect to the molecular monolayer adsorption properties on metallic substrates. Namely we address the evidence that the presence of a *d*-metal ion in the macrocycle drives the molecule-substrate interaction inhibiting the possible conformational change easily obtained by annealing the free-base molecules. We also demonstrate, using high-resolution X-ray spectroscopy supported by density functional theory calculations, that 2H-tetraphenylporphyrins metalate at room temperature by incorporating a surface metal atom when a (sub)monolayer is deposited on 3d magnetic substrates, like Fe(110) and Ni(111) [5].

These methods indicate novel ways to form, via chemical modification and supramolecular engineering, metal-organic networks on magnetic substrates with an intimate bond between the macrocycle molecular metal ion and the substrate atoms.

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#### #437 - Toward efficient OLED lighting: the key role of crystal structure in enhancing FIrpic phosphorescence

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Researchers usually endorse amorphous films with respect the crystalline-ones in fabricating organic light-emitting diodes. In spite of this, here we report a singular electro-optical behaviour of sky blue phosphorescent OLEDs (PHOLEDs), incorporating crystal structures of bis(4',6'-difluorophenylpyridinato)-iridium(III) picolinate (FIrpic) opportunely dispersed inside a 4,4',4''-tri(N-carbazolyl)-triphenylamine (TCTA) matrix. The specific molecular arrangements that lead to the molecular crystal formation provide a widening of emission spectrum, higher carrier mobility, higher exciton recombination yield and increased material stability. Consequently, the electro-optical characteristics of sky-blue PHOLEDs are optimized: we underline the unexpected ability of crystalline FIrpic to reduce the efficiency roll-off at high operating luminance with respect conventional p-i-n sky-blue PHOLEDs: from 6.000 to 26.000 cd/m<sup>2</sup> we report a minimal efficiency roll-off of 2 cd/A.

These results lead to a full employment of FIrpic crystal structure in two colours (sky-blue and orange)-based WOLED for lighting or other high luminance applications up to 10000 cd/m<sup>2</sup> where, to our knowledge, the power efficiency falls down close to zero.

Particularly, we report a power efficiency of around 20 lm/W at 1000 cd/m<sup>2</sup>, that gradually rolls down up to 13,5 lm/W at 10000 cd/m<sup>2</sup>, with an excellent CRI of 76.

**#438 - Elementary excitations in carbon nanotubes**

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Carbon nanotubes have been considered for several years as band like semiconductors whose frontier states are well described by a single particle picture, supporting electron and hole as elementary excitation photogenerated by a band to band optical transition. A wealth of experimental and theoretical results have however pushed forward the importance of Coulomb correlation and excitonic effects. A smooth transition thus occurred in the community, from thinking at carbon nanotubes as band semiconductors to considering them as excitonic semiconductors. This well accounts for a number of observations, like optical properties, yet many phenomena remains puzzling, as for example the efficient charge photogeneration in neat materials free from "intended" dissociating interfaces. By a careful interpretation of the transient spectra, we are able to show that indeed both charge carriers and excitons are to be considered in order to fully capture excitation dynamics in carbon nanotubes. In particular following photoexcitation we find a consistent signature of Stark shift of the excitonic levels that is assigned to the generation of charge carriers whose dynamics are characteristic in 1D.

**#439 - CVD of 1D&2D nanomaterials: from model systems to integrated processing**

Stephan Hofmann (I) - University of Cambridge

Chemical vapor deposition (CVD) has become the dominant technique for carbon nanotube (CNT) growth over the last two decades, and due to its versatility and scalability, CVD is currently also becoming the method of choice for the industrial materials development of 2D materials. Essential to growth control for 1D and 2D material CVD is an understanding of the underlying growth mechanisms, specifically the interactions of the precursors and growing structure with the catalyst.

We systematically use in-situ characterisation techniques, ranging from environmental scanning and transmission electron microscopy (ESEM/ETEM) to high-pressure X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD), combined with process development for a range of industrial reactors to reveal some of the key mechanisms for the scalable CVD and device interfacing of these nanomaterials. Here we present our latest results, including insights into the dynamics of the graphene-catalyst interaction [1], phase control for nanoparticulate Fe catalysts during CNT CVD [2] and rational catalyst design for compound 2D materials, such as h-BN [3,4].

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**#440 - Interfacing nanomaterials to excitable cells: a new family of bio-hybrids exploiting carbon-based material.**

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Neurobiology increasingly endeavours combining material science, nanotechnology and cell biology to engineer hybrid constructs where a cellular phase and a synthetic phase are merged together and promote novel function to complex biosystems. Carbon nanotubes (CNTs), due to their physicochemical properties, have played a key role in this contest. With proven *in-vitro* and *in-vivo* cellular biocompatibility [1] and the ease of immobilisation on virtually every surface, CNTs possess the ability to interact intimately with neuronal membranes leading to the emergence of a hybrid organic/inorganic interface between cells and CNTs ultimately responsible of boosting neuronal activity [2].

This powerful symbiosis, although not entirely understood in its mechanisms, is presumably facilitated by the good matching of CNTs' (nano)dimensionality with cells' membrane or cytoskeletal constituents (e.g. actin and tubulin filaments). The most surprising point is the ability of this local interaction to be translated into cues driving the entire synaptic network development [3] system.

Here we exploit the ability to grow CNTs in form of patterns of any arbitrary shape and dimension on a supporting surface in addition to that of decorating by CNTs the surface of complex supporting scaffolds to create innovative hybrid interfaces, in both

2D and 3D fashion. CNT interfaced neurons were characterised in morphology via electron microscopy (EM) and histochemistry while network functionality was described in terms of activity via calcium imaging analysis. The establishment of a hybrid, CNT coupled, neuronal network opens, for the first time, to the possibility to develop new composite systems where organic and inorganic phases will cooperate together to carry out novel effective functionalities. By a parallel approach we investigated cell-membrane interactions with the artificial materials, to address the core mechanisms instructing cell behaviours. In particular, we used our previous knowledge on nanomaterials and neurons to engineer novel devices towards unconventional neuro-medicine applications.

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#### #441 - Carbon nanotube based platforms for gas sensing and photon harvesting

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In spite of the huge number of publications on devices and applications, carbon nanotubes (CNT) are still attracting a large interest in the field of gas sensing and photon harvesting. In the former case, CNT-based chemiresistors have shown to be sensible to low ppb concentrations of target gas molecules, which make them quite attractive for low-cost diffuse environmental monitoring applications [1-3]. In the latter case, the role of CNT in PV cells has gone far beyond that of channels for an efficient transport of photogenerated carriers, as they are a component (usually the p-side) in the heterojunctions with semiconductors [4,5] or metal oxides. In this presentation it is shown how the combination of both functionalities is within reach, disclosing a rich scenario of possible applications where the absorption of gas molecules can be affected by internal fields arising at the junction and, conversely, PV cells efficiencies can be driven by the absorption of selected molecules.

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#### #442 - Solvatochromic properties of fluorescent carbon nanodots

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Carbon nanodots (CDots) are an interesting class of zero-dimensional nanomaterials discovered in 2004. They consist in spherical particles with sizes in the range 1-10 nm, mostly constituted by Carbon, Oxygen, Hydrogen. The core of CDots is usually rich of carbon and can be amorphous or crystalline, while their plentiful surface groups, mostly associated to carbon oxidation, strongly depend on the synthetic method used to create the nanoparticles. The growing interest on CDots is due to their unusual and appealing features, particularly their intense and tunable photoluminescence, combined with nontoxicity and biocompatibility. The mechanisms behind CDots photoluminescence are still debated: many processes have been proposed to be the source of light emission, but the matter is still unsettled.

In our study, CDots produced by microwave-induced decomposition of organic precursors are found to be very soluble in polar solvents such as water, alcohols, acetonitrile, and virtually insoluble in apolar media. Hence we have studied their optical absorption and fluorescence properties when dispersed in solvents with different dielectric constants and/or hydrogen bond capabilities, in order to better understand their emission mechanisms and to investigate their sensitivity to different environments. In fact, solvation can cause notable changes in photo-physical properties through the interactions between the solvent and the emitting fluorophores.

We find that the lowest-energy electronic transitions of CDots, responsible of their fluorescence, stem from two distinct chromophores which are both sensitive to solvent polarity and H-bonding capability. In fact, the fluorescence quantum yield, the decay lifetime and the fluorescence peak energy are all affected by the dielectric constant of the solvent they are dispersed in. In addition, modifications are observed depending on whether the solvent is protic or aprotic, highlighting a role of H-bonding

interactions between the solvent and the surface of CDots. Overall, these data provide strong evidence that the emitting transitions of these CDots are associated to surface moieties, and allow drawing conclusions on the microscopic properties of the emitting chromophores.

#### #443 - Advanced transmission-electron-microscopy investigations of inductive plasma torch synthesized silicon nanowires

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Nanoscience and nanotechnology have emerged as one of the major mark of the scientific and technological development in the past few decades. In this contest, nanostructure synthesis and characterization constitute the crucial steps to explain nanostructure formation from a fundamental point of view in order to adapt the nanostructures to the desired applications.

We report on an original and high throughput (~Kg/day) induction plasma torch based process for the synthesis of Si NWs. Transmission Electron Microscopy turns out to be a powerful tool for a full material characterization as well as for the comprehension of the growth mechanism of Si nanowires (NWs). HR-TEM, Energy Filtered-TEM and STEM-EDX were combined in order to perform an accurate study of the nanomaterials (1-10 nm size range) from the morphological, structural and chemical point of view. The as-synthesized material consists of a mixture of SiNWs and Si nanospheres. We found that Si NWs formation comes from two competitive growth mechanisms, namely Vapor-Liquid-Solid mechanism and Oxide Assisted Growth (OAG). In detail, Si NWs grown by OAG present an intriguing structure formed by a nanometric cylindrical or "pearl necklace" Si core covered by a SiO<sub>2</sub> shell, making them extremely interesting for optical applications.

#### #444 - SILICON NANOWIRE FORESTS FOR ELECTROCHEMICAL BIOSENSORS

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Nanomaterials, such as metallic or oxide nanoparticles, carbon nanotubes, graphene and semiconductor nanowires, are emerging as new platform of highly performing sensors for label-free detection of biological species. Among all these nanoscale materials, silicon nanowires (SiNWs) offer a series of advantages including their full compatibility with the well-established silicon technology. Recently, ultrasensitive SiNW sensors based on field-effect transistors (FETs) have been demonstrated for the detection of ions, small molecules, proteins, DNA and viruses. The SiNW-FET consists of single or few SiNWs, prepared as single-crystal and doped structures, which are connected to source and drain electrodes by forming the active channel whose conductivity changes in response to molecular recognition. For effective devices, electrically addressable array of NW FETs should be developed. This requires a fine control of the fabricated structure as well as the use of sophisticated and complex technological processes, which are affected by important drawbacks such as the high costs, the low throughput capability and scalability. To overcome these limits, which would confine the use of SiNWs in niche applications, we propose a change of the approach by exploiting for sensing purposes very dense, disordered and randomly oriented ensemble of Si NWs, i.e. SiNW forest. These materials allow indeed the use of fabrication techniques already implemented in industrial processes, such as Plasma Enhanced Vapor Deposition (PECVD) and conventional lithographic technology. The main idea is to investigate if it is possible to reach high sensing performance by exploiting the peculiar morphology of these systems, which offer a macroporous framework easily to functionalize and accessible by analyte molecules. This approach requires the control of the morphological characteristics and surface modifications over an ensemble of disordered NWs rather than over individual elements within ordered array.

For this purpose we fabricated three-electrode impedance devices with a working electrode (WE) formed by a forest of SiNWs, 1-2micron long, covered by a thin layer (150 nm) of Au (Au/SiNWs), a ring-shaped Au counter electrode (CE) and an Ag/AgCl reference electrode (RE). The devices were fabricated by PECVD at low temperature (350°C) on polyimide membrane. To explore the biomolecular sensing capability of these systems, we functionalized the Au/SiNW WE with biotin and studied the well-known ligand-receptor binding of biotin-avidin. Impedance measurements showed an efficient detection of the avidin over a wide range of concentrations from micromolar down to the picomolar values.

**#445 - Dimer Aggregation and Confinement for Ultrabright Fluorescence in Dye Doped Hexagonal Ordered Mesoporous Silica Nanoparticles**

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Fluorescent micro and nanoparticles find applications in a wide range of fields, from biomedicine as probes for tagging and labeling, in particular for super-resolution fluorescence microscopy, to photonics as active medium for nanolasing. Among the others, silica nanoparticles are a suitable host for fluorescent elements because of its bio-compatibility and ease of functionalization. For instance, hexagonal arrangement of one or two-dimensional mesopores with diameters ranging from 2 to 10 nm (MCM-41) allows high surface area and good thermal stability, which make them an attractive molecular sieve for catalysis, sensor applications, or quantum confinement of guest molecules. Dye doped silica nanosized systems were largely studied in the past in the attempt to solve two main difficulties: the concentration phenomenon and the leaching effect. In this work the fluorescence properties of Rhodamine 6G (Rh6G) doped silica nanoparticles prepared by a one-pot templated base-catalyzed sol-gel self-assembly method are discussed in terms of concentration and leaching effects. To solve these typical drawbacks of silica based organic-inorganic hybrid and exploit the formation of aggregates to achieve super fluorescence, a new sealing approach was tested, where the applied surfactant plays both the role of sealant and splitting element to control both the aggregation and the confinement of the dyes. Indeed structural and morphological analysis showed that we were successful in synthesizing hexagonal ordered mesoporous silica nanoparticles of about 130-160 nm in diameter with pores in the 2-3 nm range. In addition, depending on the rinsing treatment, an external silica shell of about 1-2 nm was observed in some system allowing efficient confining of dye molecules within the host matrix. Indeed dye leaching was tested against water and alcohols showing a larger resilience to leaching by water rinsing, a quite high quantum yield despite the large dye concentration (40-50%) and an outstanding brightness given by thousands (up to  $10^4$ ) of emitting molecules per nanoparticle.

**#446 - Silicon Nanowires Random Fractal Array: striking optical performances towards new fascinating physical phenomena**

Barbara Fazio (I) - CNR - IPCF Messina

Semiconductor nanowires (NWs) have attracted a considerable interest within the scientific community as innovative materials for applications in light sources sensing and nano-scale photovoltaic devices. The optimization of NWs dimensions and the spatial arrangement in novel textured materials, both ordered and disordered, play a key role on the transport of the light towards striking optical performances based on light trapping, multiple scattering and localization of light. In particular, a fractal arrangement represents the case of a material with a complex disorder and strong structural heterogeneities correlated at all length scales. Furthermore, the property of dilation symmetry and the lack of translational invariance lead these systems to spatially localize the running waves. Since silicon is the most important and well known semiconductor, because silicon-based devices have dominated microelectronics for many decades, a winning strategy both for solar cells and photonic devices applications is the realization of a random fractal structure of silicon nanowires as unique material that meets all the previous demands. Here we present the impressive optical properties of a forest of ultrathin vertically aligned silicon nanowires arranged in a 2D fractal array realised without the use of mask or lithography process. This kind of structure allows for a particularly high efficiency of light trapping in all the visible range reaching values of total reflectance below 1%. Furthermore, the black-body behaviour and the occurrence of strong in plane multiple light scattering are responsible for an enhanced optical emission in terms of Raman scattering and photoluminescence, paving the way towards a new class of silicon devices. Moreover, the random organization and the strongly scattering performances allowed for the observation of novel fascinating physical phenomena as the evidence of interference effects in spontaneous Raman scattering.

**#447 - Silicon Nanowires: from Synthesis to Photonic Applications**

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Semiconductor nanowires (NWs) are attracting the interest of a large scientific community as building blocks for a wide range of future nanoscaled devices. In this work we show that metal-assisted chemical etching of Si substrates is a powerful technique to obtain nanometer-size, high density and low-cost Si NWs with high and controllable aspect ratio. NWs obtained by this technique maintain the same structure and doping of the starting substrate and exhibit a very bright room temperature photoluminescence (PL) in the visible range, which is tunable with NWs size, in agreement with the occurrence of quantum confinement effects. Light

emitting devices based on Si NWs, showing an efficient room temperature electroluminescence (EL) emission at low voltage, have also been realized. This synthesis method can also be applied for the synthesis of NWs with different composition, in fact we reported the realization of Si-Ge NWs obtained from a Si-Ge multilayer. This Si-Ge NWs system represents a very attracting double emission wavelength material that operate both in the visible range and in the infrared (IR) due to the presence of quantum confined silicon and germanium. We also realized a room temperature operating hybrid light source by coupling Si NWs and carbon nanotubes (CNT). This system exhibits a double emission in the visible range from Si NWs and in the IR from CNT; a detailed study of the PL properties has been performed, and the conditions leading to the prevalence of the visible or of the IR signal have been identified.

#### #448 - Gamma - Ga<sub>2</sub>O<sub>3</sub> nanocrystals in germano-silicate glass as multipurpose photonic material

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The ability to incorporate crystalline nanostructures in amorphous glass is a successfully strategy for the design of novel functional and structural materials. On the one hand, the oxide matrix ensures ideal workability, chemical inertness, and mechanical robustness. On the other hand, crystalline nanoparticles may give rise to unprecedented optical, electrical, or mechanical behaviour. In this view, alkali germano-silicate glasses containing  $\gamma$ -Ga<sub>2</sub>O<sub>3</sub> nanoparticles, prepared by the melt-quenched method, represent an interesting solution as multipurpose photonic materials. In fact, the low refractive mismatch between crystals and matrix as well as the ability of obtaining nanostructures with dimensions of the order of few nanometers enables the possibility of having a transparent material with peculiar optical properties.  $\gamma$ -Ga<sub>2</sub>O<sub>3</sub> is indeed a wide-band gap semiconductor ( $E_G = 4.9$  eV) showing strong blue luminescence upon excitation at wavelength shorter than 280 nm and related to recombination at donor and acceptor pairs. For these reasons Ga<sub>2</sub>O<sub>3</sub>-based materials would be particularly suitable, in principle, for the fabrication of simple and robust UV-to-visible converters. The photoluminescence excitation threshold at 280 nm coincides with the UV-C region above which the solar spectrum does not give any background to the detection of UV-emitting events such as flames, electric sparks, and corona dispersions, which can significantly affect safety conditions in working places, energy-saving, and electric power distribution reliability. Beyond this intrinsic luminescence,  $\gamma$ -Ga<sub>2</sub>O<sub>3</sub> may also host other optically-active ions so as to enrich the photophysics of the system. Here we present our recent results on the optimization of the intrinsic emission features of these glassceramics and their application as UV-light converter in solar-blind passive devices. Moreover, we also discuss the optical behaviour of samples doped with rare-earth and transition metal ions. In particular, we will focus on samples doped with Nickel ions that show strong broadband infrared emission, and Gadolinium doped samples where energy-transfer processes take place thus enabling rare-earth emission with large excitation cross section.

#### #449 - Critical Casimir assembly of quantum dots

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A major challenge in the development of highly efficient semiconductor quantum dot-based solar cells is controlling the energy transfer between adjacent nanocrystals. This is partly due to the lack of precise, yet large-scale, control in nanoscopic dimensions, which is required to achieve a close packed and uniform superstructure [1]. We study the assembly of quantum dots in a binary mixture which exhibits temperature dependent solvent fluctuations [2]; remarkably, these induce reversible assembly even at the nanoscale. This technique allows us to finely tune the distance between the dots by simply playing with the temperature and the Debye screening length in the solution. By doing so, we observe the spectral fingerprint of inter-dot coupling as the nanostructure grows with time.

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#### #450 - Radiation Response of Optical Fibers Loaded with Molecular Oxygen

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We report an experimental investigation regarding the radiation response of Pure-Silica-Core (PSC) and F-doped Optical Fibers (OFs) previously subjected to a high pressure O<sub>2</sub> loading thermal treatment.

First, by micro-Raman spectroscopy we demonstrate the efficiency of the O<sub>2</sub> loading technique we applied. In particular, we showed that high concentrations ( $\sim 2 \cdot 10^{18}$  molecules/cm<sup>3</sup>) of molecular oxygen are incorporated in the whole OF cross section, almost reaching a saturation condition of the samples. Afterwards, we studied the effects of the O<sub>2</sub> loading treatment on the radiation response of the OFs. For this purpose we carried out a comparative study based on simultaneous online Radiation Induced Attenuation (RIA) measurements of the O<sub>2</sub> loaded and unloaded OFs in the UV-Visible spectral domain [1]. The experiments were performed by irradiating with 10 keV X-rays. The RIA spectra clearly show a strong impact of the O<sub>2</sub> excess. The loading treatment causes an increase of the radiation sensitivity of the OFs in the UV-Visible domain. The presence of radiation induced interstitial ozone molecules is also inferred by decomposition of the RIA spectra. The information gained with the RIA experiments is further supported by Electron Paramagnetic Resonance measurements performed on  $\gamma$ -irradiated samples. As a radiation hardening effect it is found that the irradiation induces a ten time lower concentration of E'(Si) centers in the O<sub>2</sub>-loaded OFs.

Another interesting phenomenon detected in the O<sub>2</sub>-loaded OFs is related to an infrared Radio-Luminescence (iRL) of O<sub>2</sub> molecules: a sharp luminescence at 1272 nm was indeed detected during irradiation by 10 keV X-rays [2]. We will focus on the applicative aspects related to this effect: the results we obtained show that the iRL is stable up to doses of 1 MGy(SiO<sub>2</sub>) and is linearly dependent on the dose-rate up to the maximum investigated dose-rate of  $\sim 200$  kGy(SiO<sub>2</sub>)/h. On the basis of the obtained results we suggest that the iRL can be exploited for real-time, remote dosimetry in environments characterized by high radiation doses and high dose-rates.

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#### #451 - Luminescence of Si/SiO<sub>2</sub> Nanostructures produced by Laser Ablation in Water

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Miniaturization of Silicon down to nanoscale induces a visible photoluminescence (PL) surprising for a material which is weakly emissive in the bulk form. Due to quantum confinement effects, the smaller the Si nanocrystals (Si-nc) are, the more the PL is shifted towards the blue range. This feature has attracted a wide interest motivated by the use of Silicon-based nanomaterials in several applications (optoelectronics, photovoltaics, bioimaging). A great effort is currently devoted to develop production methods successful both to tune the luminescence and to enhance the brightness of Si-nano emitters. Laser ablation (LA) in liquids is particularly powerful since it is a green method suitable for biological applications and it provides effective control parameters (laser photon energy, fluence, pulse duration, liquid reactivity) for the morphology and the structure of the related products.

The purpose of this work is the study of nanosized materials produced by Nd:YAGLA of a Si wafer in deionized water. The investigation has been carried out by combining complementary techniques to probe morphological, structural and optical properties. Transmission electron microscopy (TEM) images and energy-dispersive X-ray spectroscopy (EDXS) analysis reveal Si-ncs and amorphous SiO<sub>2</sub> nanoparticles produced by Si oxidation in water. IR absorption and Raman scattering evidence as well vibrational features characteristic of these nano-materials. Time resolved luminescence spectra under a tunable laser excitation allow to highlight different emissions. SiO<sub>2</sub> nanoparticles show a band around 2.8 eV ( $\tau \sim 5$  ns) related to surface states and two bands at 4.4 eV ( $\tau \sim 5$  ns) and at 2.7 eV ( $\tau \sim 10$  ms) associated with oxygen deficient centers. Si-ncs are characterized by a luminescence band around 1.9 eV with lifetime  $\tau \sim 10$   $\mu$ s. We have also evidenced that this emission is influenced by the pH of the solution: its intensity and its lifetime increase by a factor 3 when the pH is less than 4. This finding points out that the hydrogen controls the surface chemistry at the Si/SiO<sub>2</sub> interface favoring the increase of the emission efficiency.

#### #452 - Tunable visible light emission from Eu-doped SiOC thin films

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In recent years, rare earths (REs) doped inorganic materials have been widely applied in lighting, display devices and photonics. In these fields an important role has been played by phosphors. Most of the phosphors used are REs-doped oxide or sulfide-based materials; among the different REs, a particular interest has been devoted to Eu, which has the peculiar characteristic to be stable both in its divalent and trivalent oxidation states. In particular, emission of  $\text{Eu}^{2+}$  is quite strong (being due to electric dipole allowed transitions) and is characterized by a broad peak in the wavelength range 400-600 nm.  $\text{Eu}^{3+}$  emission, instead, presents several sharp peaks at around 600 nm whose intensity is low, being due to electric-dipole forbidden transitions. These peculiar optical properties make Eu-based materials very promising candidates not only for the fabrication of light sources and displays, but also for applications in photonics, especially if we would be able to obtain an efficient light emission from an Eu-doped Si-compatible host matrix.

In this work SiOC thin films, doped with different Eu concentrations, have been synthesized by RF magnetron co-sputtering. Optical properties of these films have been investigated by photoluminescence (PL) and cathodoluminescence (CL) measurements. In both cases a very bright  $\text{Eu}^{2+}$  light emission in the 400-600 nm range has been obtained. We were able to achieve this wide range by properly changing the Eu concentration in the thin films. In addition, bilayers consisting of two SiOC films doped with different Eu concentrations have been synthesized and investigated. We have demonstrated that for the bilayer, a proper choice of the annealing temperature allows to avoid Eu diffusion and clustering and to obtain an intense PL white emission at room temperature, characterized by a color rendering index higher than 90. Furthermore, CL measurements have demonstrated that by properly varying the electron beam energy it is possible to control at the nanoscale the electron penetration depth inside the bilayer, thus obtaining a depth-resolved CL, with a continuous tuning of the emission from 400 to 600 nm.

The very efficient room temperature PL and CL signals and the compatibility of the SiOC films with Si technology, open the way to new and promising applications of Eu-based materials in lighting, display technology and photonics.

#### #453 - First-principles investigation of paramagnetic centers in v-SiO<sub>2</sub>, Ge-doped SiO<sub>2</sub> and v-GeO<sub>2</sub>.

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We present a first-principles investigation of paramagnetic centers in vitreous silica (v-SiO<sub>2</sub>), Ge-doped silica and vitreous germania (v-GeO<sub>2</sub>). An improved understanding of these paramagnetic defects is expected to have an impact in several scientific and technological fields ranging from silica-based optical fibers to future Ge-based microelectronic devices [1,2].

We generate and analyze a large number of defect configurations that allow us to discuss structural models of the E' centers in v-SiO<sub>2</sub> [3] and of the Ge-E', Ge(1) and Ge(2) centers in Ge-doped silica and v-GeO<sub>2</sub> [2,4]. In particular, we provide evidence for an assignment of the Ge(2) center to Ge forward-oriented configurations, analogously to the E'alpha center in silica [2-4], leading to an updated and unified picture of the defects in pure v-SiO<sub>2</sub>, v-GeO<sub>2</sub> and Ge-doped SiO<sub>2</sub>.

We discuss the Ge(2)/E'alpha precursor issue by showing that once a two-fold Ge (i.e. a GLPC center) or a twofold Si is ionized it can easily relax and give rise to a forward-oriented configuration i.e. a Ge(2)/E'alpha center. Furthermore we discuss the interconversion mechanisms between several defect configurations, and in particular we show that twofold Ge (and twofold Si) configurations can be generated from Ge-Si (and Si-Si) dimer configurations by overcoming rather small energy barriers.

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**#454 - Diamond-based single-photon emitters***Paolo Olivero (I) - Università di Torino*

Diamond is an extreme material not only in its structural and electrical properties, but also with respect to the extremely vast range of optically active color centers that can be hosted in its structure: literally hundreds of different defect/impurity-based complexes emitting light from the far infra-red to the near ultra-violet have been identified so far in its crystal lattice, which is transparent over a broad spectral range. When isolated at the single-defect level, some of these "color centers" demonstrated unique properties (optical stability, quantum efficiency, convenient electronic transitions) at room temperature, that make diamond a promising choice as a stable and reliable single-photon emitter for applications in quantum communication and quantum computing.

In this talk, an overview will be given on the activities carried at the University of Torino (in close collaboration with the National Institute of Nuclear Physics - INFN and the National Institute of Metrologic Research - INRiM) on the creation and characterization of different types of color centers in artificial single-crystal and nanocrystalline diamond. In particular, the formation of color centers via MeV ion implantation will be discussed, as well as the quantum-optical characterization in single-photon emission regime of nitrogen-vacancy complexes and other novel NIR-emitting color centers.

**#455 - Giant excitonic effects in Graphene-like 2D systems***Olivia Pulci (I) - Dept. of Physics University of Rome Tor Vergata, ETSF, and MIFP*

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The electronic and optical properties of 2D systems are here investigated by ab-initio (DFT, GW and BSE approaches) and model methods [1,2]. We demonstrate that the infrared absorbance of Dirac systems such as Graphene, Silicene, and Germanene tends towards a universal value proportional to the fine structure constant [3]. Optical and energy loss spectra are also presented and discussed as fingerprints for counting the number of layers.

Functionalizing these systems with Hydrogen opens a gap and induce huge excitonic effects [4] that we study by ab-initio methods and with a simple 2D excitonic model beyond the 2D-Hydrogen approximation [1,2]

Finally, we present a preliminary study of the electronic and optical properties Nitride-based 2D materials (BN, GaN, InN, AlN). Stable honeycomb structures graphene-like are found, with no buckling. Due to the different electronegativity of III and V atoms, a charge transfer occurs and a gap opens, so no Dirac cone is found in these 2D materials [5].

Confinement effects together with reduced 2D screening strongly enhance excitonic effects, creating electron-hole pairs with large (-eV) binding energy and tunable optical gap, making these materials good candidates for novel optoelectronic devices also in the THz region.

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**#456 - Advances in holographic three-dimensional particles tracking***Pasquale Memmolo (I) - Center for Advanced Biomaterials for HealthCare@CRIB, Istituto Italiano di tecnologia*

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In the last decade, digital holography (DH) in microscopy has become an high-throughput imaging instrument able to furnish a diagnostic tool for bio-microfluidic at lab-on-chip scale [1]. Among others features, DH allows accurate retrieving of the positions of multiple particles performing three-dimensional (3D) tracking, exploiting the uniqueness of the DH to provide a *posteriori* quantitative multi-focus capability and phase-contrast imaging. Several methods have been proposed to apply DH to track particles [2] as well as cells [3-5]. Holographic tracking approaches are implemented by performing two main steps, (i) the numerical refocusing [6,7] through amplitude reconstruction's contrast analysis, that permits the calculation of optical axis position of particles, and (ii) the evaluation of lateral displacements of refocused particles through quantitative phase images analysis by using suitable image segmentation methods [4]. Non-conventional holographic particles tracking methods are enveloped to calculate simultaneously all the three coordinates, i.e. without decoupling the amplitude and phase contributions of the complex wavefronts [5]. Thanks to the incredible development of such holographic-based tracking approaches, DH is increasingly used for the investigation of cells migration as well as the full morphometric characterization of biological samples, due to its capability to perform quantitative imaging of biological samples. Here, we review different holographic tracking methods, developed by our

research group in the last years [2-5], and their application to investigate the 3D particles motility in different experimental conditions.

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### #457 - Lateral heterojunctions on GdAg<sub>2</sub> surface alloy

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A two dimensional GdAg<sub>2</sub> surface alloy layer is formed exposing the surface of Ag(111) to gadolinium atoms. Due to lattice mismatch with the supporting substrate this alloy forms moiré patterns with different periodicities. These result from minute relative reorientations of the alloy layer with respect to the Ag(111) surface and of different in-layer strain [1, 2]. Although formed by the same chemical structure and composition, the moiré patterns show surprisingly distinct electronic properties. Combining scanning tunneling microscopy and spectroscopy, we will explain the relation between the electronic properties and the layer structure. Density functional theory calculations have been performed to predict the electronic properties of this alloy as the band structure, work functions and spin-orbit coupling strengths. The reason for the striking difference in the electronic properties will be explained in terms of inlayer coupling strength of the Gd atoms in the alloy and their coupling with the underlying Ag substrate. A comparison with the GdAu<sub>2</sub> alloy grown on Au(111) layer, whose electronic and magnetic structure show almost no dependence with the more periodicity [3], will be presented.

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### #458 - SILICON NANOWIRE FORESTS FOR ELECTROCHEMICAL BIOSENSORS

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Nanomaterials, such as metallic or oxide nanoparticles, carbon nanotubes, graphene and semiconductor nanowires, are emerging as new platform of highly performing sensors for label-free detection of biological species. Among all these nanoscale materials, silicon nanowires (SiNWs) offer a series of advantages including their full compatibility with the well-established silicon technology. Recently, ultrasensitive SiNW sensors based on field-effect transistors (FETs) have been demonstrated for the detection of ions, small molecules, proteins, DNA and viruses. The SiNW-FET consists of single or few SiNWs, prepared as single-crystal and doped structures, which are connected to source and drain electrodes by forming the active channel whose conductivity changes in response to molecular recognition. For effective devices, electrically addressable array of NW FETs should be developed. This requires a fine control of the fabricated structure as well as the use of sophisticated and complex technological processes, which are affected by important drawbacks such as the high costs, the low throughput capability and scalability. To overcome these limits, which would confine the use of SiNWs in niche applications, we propose a change of the approach by exploiting for sensing purposes very dense, disordered and randomly oriented ensemble of Si NWs, i.e. SiNW forest. These materials allow indeed the use of fabrication techniques already implemented in industrial processes, such as Plasma Enhanced Vapor Deposition (PECVD) and conventional lithographic technology. The main idea is to investigate if it is possible to reach high sensing performance by exploiting the peculiar morphology of these systems, which offer a macroporous framework easily to functionalize and accessible by analyte molecules. This approach requires the control of the morphological characteristics and surface modifications over an ensemble of disordered NWs rather than over individual elements within ordered array.

For this purpose we fabricated three-electrode impedance devices with a working electrode (WE) formed by a forest of SiNWs, 1-2micron long, covered by a thin layer (150 nm) of Au (Au/SiNWs), a ring-shaped Au counter electrode (CE) and an Ag/AgCl reference electrode (RE). The devices were fabricated by PECVD at low temperature (350°C) on polyimide membrane. To explore the biomolecular sensing capability of these systems, we functionalized the Au/SiNW WE with biotin and studied the well-known ligand-receptor binding of biotin-avidin. Impedance measurements showed an efficient detection of the avidin over a wide range of concentrations from micromolar down to the picomolar values.

#### #459 - Catalyst-free growth of InAs nanowires on Si(111) by chemical beam epitaxy

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We propose and investigate a new growth mechanism which yields catalyst-free InAs nanowires on Si(111) substrates by employing the chemical beam epitaxy technique. Our growth protocol consists of a low temperature nucleation and a high temperature growth steps. This method produces non-tapered InAs nanowires with controllable lengths and diameters. We show that InAs nanowires evolve from the islands formed during the low temperature nucleation step and truly grow catalyst-free, without any indium droplet at the tip. The impact of different growth parameters on the nanowire morphology is systematically investigated. In particular, a good control over the nanowire aspect ratio is demonstrated. A better understanding of the growth process is obtained through the development of a theoretical model which combines the diffusion-induced growth scenario with some specific features of the catalyst-free growth mechanism, along with the analysis of the V/III flow ratio influencing the material incorporation. As a result, we perform a full mapping of the nanowire morphology versus the growth parameters which sheds more light on the self-induced formation of III-V nanowires on silicon in general.

#### #460 - A general framework for the kinetics of progressive breakdown in MOS with Si and III-V substrates

Salvatore Lombardo - CNR-IMM

Other Authors: Felix Palumbo (CONICET, Buenos Aires, Argentina), Moshe Eizenberg (Technion, Haifa, Israel)

Gate oxide breakdown (BD) is a critical issue for advanced CMOS circuits. CMOS evolution has been driven by aggressive device scaling, the introduction of new materials such as strained Si, high-k dielectrics and metal gates, new device structures such as FINFETs, tri-gate FETs, and UTBSOI FETs, associated with a slower decrease of the supply voltages. This has resulted in an increase of the electric fields applied to the structures, resulting in improved performance but with some negative effects. Among these is the continuous increase of the tunneling current flowing across the gate oxides under circuit operation. In fact, it has been shown that such a tunneling current through the gate dielectric is the main origin of the degradation leading to BD.

Thus, dielectric breakdown is an important reliability issue on such novel device structures. The study of BD is mostly performed by using accelerated constant voltage stresses by applying a relatively large voltage difference between the gate and the source, drain, and body short-circuited together. The typical evolution of the gate current during a constant voltage oxide stress shows two distinct stages: initial defect generation and progressive BD.

Understanding the growth rate of the gate current during progressive BD is critical for projecting the long term reliability of circuits which do not fail at the onset of progressive BD but rather when the progressive BD current grows to a leakage level that causes circuit disruption. In this paper we investigate some general features of dielectric breakdown of ultra-thin gate oxides for CMOS. We discuss III-V devices with high-k/metal gate, and compare to more classical structures with silicon substrates, SiO<sub>x</sub>N<sub>y</sub> or high-k as gate dielectrics, and poly-Si or metal gate. A model of the breakdown growth dependence on voltage, temperature, oxide thickness, etc., is eventually discussed and compared to data.

We show which parameters control the breakdown growth rate providing a physical model of BD growth and comparing it to examples in a number of gate dielectrics. Such understanding may allow further improvement of reliability margins of CMOS circuits by choosing a correct combination of voltage, thickness, and thermal conductivity of the gate dielectrics.

**#461 - Phase behavior and gelation of DNA nanostars. A numerical and experimental study**

*Francesco Sciortino (I) - Dip. Fisica, Sapienza Universita' di Roma*

Colloidal particles with directional interactions are key in the realization of new colloidal materials with possibly unconventional phase behaviors. We exploit DNA self-assembly to produce bulk quantities of DNA-nanostars with three or four sticky terminals, mimicking molecules with limited valence. Theory and simulations predict that a different route to gelation becomes available when the valence of each colloidal particle is suitably reduced: gelation should be achievable through a reversible sequence of equilibrium states. With experiments and simulations we show that as temperature is decreased, the relaxation time for density fluctuations slows down by about five orders of magnitude, following an Arrhenius scaling in the entire experimentally accessible temperature window. The system is in thermodynamic equilibrium at all temperatures. We finally show that DNA hydrogels provide a striking example of ultrastable liquids, i.e. liquids more stable than crystals.

## Relevant bibliography

Silvia Biffi, Roberto Cerbino, Francesca Bomboi Elvezia Maria Paraboschi, Rosanna Asselta, Francesco Sciortino and Tommaso Bellini

Phase behavior and critical activated dynamics of limited-valence DNA nanostars  
 Proceedings National Academy of Science, 110 15633-15637. DOI: [www.pnas.org/cgi/doi/10.1073/pnas.1304632110](http://www.pnas.org/cgi/doi/10.1073/pnas.1304632110) (2014)

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 Equilibrium gels of low-valence DNA nanostars: a colloidal model for strong glass formers  
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[5]Lorenzo Rovigatti, Francesca Bomboi, and Francesco Sciortino  
 Accurate phase diagram of tetravalent DNA nanostars  
 J. Chem. Phys. 140, 154903 (2014). <http://dx.doi.org/10.1063/1.4870467>

**#462 - The electric dance of cholesteric colloids**

*Enzo Orlandini (I) - University of Padova, Department of Physics and Astronomy*

*Other Authors: G. D' Adamo (SISSA), C. Micheletti (SISSA), D. Marenduzzo (University of Edinburgh)*

Dispersions of colloidal particles in liquid crystals are nowadays a subject of intensive studies due to their potential as novel and versatile metamaterials with important applicative avenues such as digital-ink technologies, biosensors and optical devices.

In this talk I will report theoretical results, based on lattice Boltzmann simulations, on a novel method to manipulate the spatial arrangements of colloids in cholesteric liquid crystals. By controlling the amplitude and shape of a time-dependent electric field, I will show that the system can be reproducibly driven out of equilibrium through different kinetic pathways and navigated through a glassy-like free energy landscape encompassing many competing metastable equilibria. Such states range from simple Saturn rings to complex structures featuring amorphous defect networks, or stacks of disclination loops. In particular, by using suitable non-equilibrium electric pulses, one can drive colloids from planar to linear, rope-like configurations and vice-versa.

These results can stimulate the development of new (e.g. non equilibrium) experimental procedures to control the three-dimensional patterning and self-assembly of colloidal particles suspended in complex fluids as well as prompt the design of new types of switching devices with tunable elastic and electro-optic properties.

**#463 - Relaxational dynamics in nematic liquid crystals**

Paolo Biscari (I) - Politecnico di Milano

Other Authors: Antonio DiCarlo, Dipartimento di Matematica & Fisica, Universita' di Roma Tre, Stefano Turzi Dipartimento di Matematica, Politecnico di Milano

We develop a novel hydrodynamic theory of liquids fit to bridge the gap between the fluid-like behavior typically exhibited at low-frequency regimes and the solid-like response observed at high frequencies. In the case of nematic liquid crystals the theory predicts frequency-dependent acoustic anisotropy and relaxation effects. In the hydrodynamic (lowfrequency) limit a new Parodi-like relation emerges. We present the theoretical predictions and test them against evidence from physical experiments and molecular dynamics simulations. [1] P.B., S. Turzi, A. DiCarlo: Anisotropic wave propagation in nematic liquid crystals. *Soft Matter* 10 (2014), 8296-8307. [2] P.B., S. Turzi, A. DiCarlo: Liquid relaxation: A new Parodi-like relation for nematic liquid crystals, to appear (2015).

**#464 - Orientational order and dynamics in liquids**

Bernd Ensing - University of Amsterdam

The orientational ordering and the dynamics of solvent molecules in liquids and solutions is revealed by the decay of vibrational anisotropy. We show that the functional form of this decay is determined by the (distribution of) angles between the vibrating bonds of the molecules between which energy transfer occurs, and that the initial drop in the decay reflects the average angle between nearest neighbors. We use this effect to observe the difference in local orientational ordering in the two hydrogen-bonded liquids ethanol and *N*-methylacetamide. We use forcefield and ab initio (DFT-based) molecular dynamics simulations to verify and calibrate the relation between the measured anisotropy decay and the angular distribution [1].

In aqueous solutions of amphiphilic molecules, such as urea and tetramethylurea, the mid-infrared pump-probe experiments show that the reorientation of the water molecules contains a slow component that has previously been attributed to immobilized water in contact with the hydrophobic parts of the solutes. Our simulations show that the slowdown can be understood as a difference in the balance between two (associative and dissociative) hydrogen-breaking mechanisms of solvent molecules nearby or far from the amphiphiles [2].

[1] Local orientational order in liquids revealed by resonant vibrational energy transfer

M. R. Panman, D. J. Shaw, B. Ensing, and S. Woutersen

*Phys. Rev. Lett.* 113, 207801 (2014)

[2] Slowdown mechanism of water dynamics around small amphiphiles

W. H. Brandeburgo, S. T. van der Post, E. J. Meijer, and B. Ensing

*Manuscript submitted*

**#465 - Cyclization Probabilities of Small DNA Molecules**

Marco Zoli - University of Camerino

Many experiments have demonstrated that DNA exhibits sequence-dependent bending and torsional flexibility which may have biological relevance in the DNA-protein interplay.

Such properties have been investigated by several experimental methods including gel electrophoresis, crystallography and, above all, DNA cyclization which permits to test the circularization rates of DNA sequences in the presence of ligase enzymes.

From a theoretical viewpoint, cyclization rates can be analyzed via calculation of the  $J$ - $J$  factors which are essentially given by the ratio of the partition functions of circular and linear structures.

This program is carried out in the present work by means of the path integral method for DNA [1]. The theoretical background for the application of the path integral formalism to predictive analysis of the molecule thermodynamical properties is discussed [2,3]. A model is developed to compute the helix unwinding in circular sequences with variable radius [4].

Both homogeneous and heterogeneous molecules are studied to detect the effects of the sequence specificities on the cyclization probabilities. The latter are also evaluated as a function of the sequence length.

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#### #466 - Effects of viscoelasticity on droplet dynamics and break-up in microchannels : T-Junction & Cross-Junction

Anupam Gupta - University of Rome "Tor Vergata"

Other Authors: Mauro Sbragaglia (Department of Physics and INFN, University of Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy)

The effects of viscoelasticity on the dynamics and break-up of liquid threads in microfluidic devices, i.e., T-junctions & Cross-junction are investigated using numerical simulations of dilute polymeric solutions for a wide range of Capillary numbers (Ca), i.e., changing the balance between the viscous forces and the surface tension at the interface, up to  $Ca = 10^1$ . A Navier-Stokes (NS) description of the solvent based on the lattice Boltzmann models (LBM) is here coupled to constitutive equations for finite extensible non-linear elastic dumbbells with the closure proposed by Peterlin (FENE-P model). We present the results of three-dimensional simulations in a range of Capillary numbers and flow-rate ratios which is broad enough to characterize all the three characteristic mechanisms of breakup in the confined T-junction, i.e., squeezing, dripping and jetting regimes and all the two characteristic mechanisms of breakup in the confined flow-focusing device, i.e., droplet formation at the cross-junction (DCJ) and droplet formation downstream of the cross-junction (DC). The various model parameters of the FENE-P constitutive equations, including the polymer relaxation time  $\tau_P$  and the finite extensibility parameter  $L^2$ , are changed to provide quantitative details on how the dynamics and break-up properties are affected by viscoelasticity. We will present both the cases of Droplet Viscoelasticity (DV), where viscoelastic properties are confined in the dispersed (d) phase, as well as cases with Matrix Viscoelasticity (MV), where viscoelastic properties are confined in the continuous (c) phase. Moderate flow-rate ratios  $Q \sim O(1)$  of the two phases are considered in the present study. Overall, we find that the effects are more pronounced in the case with MV, as the flow driving the break-up process upstream of the emerging thread can be largely perturbed by the polymeric stresses.

**#467 - NANOSTRUCTURED METAL HYDRIDES FOR ENERGY APPLICATIONS: STATE OF THE ART AND FUTURE TRENDS**

Luca Pasquini (I) - University of Bologna - Department of Physics and Astronomy

Metal hydrides are a fascinating class of materials that can be used for several energy applications and devices, such as hydrogen storage, heat storage, heating/cooling systems, batteries, smart solar collectors and various types of sensors. Their properties and range of applications strongly depend on the thermodynamics of hydrogen sorption, i.e. on the enthalpy / entropy changes, which dictate the equilibrium temperature and pressure for the metal-hydride transformation. In addition, the kinetics of hydrogen sorption are determined by the interplay between dissociation/recombination of the hydrogen molecule, hydrogen diffusion in subsurface and bulk layers, and nucleation of the new phase. Quite often, in order to fulfill specific application-dependent requirements, the speed of these basic mechanisms must be increased using suitable catalysts or realizing peculiar microstructures. The intensive investigation of nanostructured metal hydrides during the last decade has been driven by the ambition to tune the thermodynamics and kinetics of hydrogen absorption and release through the exploitation of several size- and surface-related phenomena. In this talk, I will present selected examples of how the thermodynamics and kinetics of hydrogen sorption can be modified through careful control over material's structure, morphology and composition at the nanoscale. In particular, I will report on the main research activities carried out within the frame of the COST Action "Nanostructured materials for solid-state hydrogen storage", a large European network launched in October 2011. Several issues related to nanostructured hydrides, from novel synthesis techniques, to advanced structural characterization with in situ capabilities, to measurements of hydrogen sorption behavior, will be presented. Particular emphasis will be given to lightweight Magnesium-based hydrides with different morphologies and composition, including nanoparticles/nanodots, thin films and multilayers, nanoconfined alloys, and core-shell structures.

**#468 - Li-S batteries characterized by operando x-ray absorption spectroscopy**

Giuliana Aquilanti (I) - Elettra - Sincrotrone Trieste

Other Authors: Iztok Arčon (University of Nova Gorica, Nova Gorica, Slovenia, Institut Jožef Stefan Ljubljana, Slovenia, Centre of Excellence Low Carbon Technologies Ljubljana, Slovenia), Manu Patel (National Institute of Chemistry Ljubljana, Slovenia), Lorenzo Stievano (University Montpellier II, Montpellier, France), Robert Dominko (National Institute of Chemistry Ljubljana, Slovenia)

Rechargeable lithium-sulfur (Li-S) batteries are actually the most promising solution for electrically driven vehicles. Advanced Li-S batteries for automotive use with high energy density, charge efficiency and durability, meeting or exceeding safety and low cost standards are being developed within the EU project EUROLIS ([www.eurolis.eu](http://www.eurolis.eu)). Operando sulfur K-edge XANES and EXAFS analysis are powerful and indispensable tools to characterize the redox chemistry, and to relate the electrochemical mechanism to the local structure behavior. Sulfur K-edge XANES spectra provide information on sulfur oxidation state and chemical bonding. Different sulfur compounds that coexist in the battery (elemental sulfur, sulfur-polysulfides and sulfur bound in electrolyte) can be efficiently distinguished, and their relative amount in the cathode can be monitored precisely during battery operation by linear combination fit of the XANES spectra.

Thanks to the use of a tailored electrolyte that did not contain any sulfur-based compound the operando sulfur K-edge EXAFS analysis of Li-S battery during electrochemical cycling is possible for the first time. This allows us to study the transformation of the local environment of the sulfur centers in the electrode and to highlight possible interactions between lithium polysulfides ( $\text{Li}_2\text{S}_x$ ) and the host matrix. In particular, the EXAFS analysis provides an accurate description of the mechanism of sulfur conversion into  $\text{Li}_2\text{S}$  in the given Li-S battery configuration.

Finally, we present the methodological approaches for efficient XAS experiments at sulfur K-edge (2472 eV) in fluorescence detection mode. The limitations and sources of potential systematic errors in sulfur K-edge XANES and EXAFS analysis due to small and strongly energy dependent penetration depth of X-ray beam and self-absorption effects in the sample are discussed.

**#469 - Plasmonic and thermoelectric properties of metal-doped ZnO transparent conductive oxides for energy conversion**

Arrigo Calzolari (I) - CNR-NANO Istituto Nanoscienze, Centro S3

Other Authors: Alessandra Catellani (CNR-NANO Istituto Nanoscienze, Centro S3, Modena IT), Alice Ruini (Universita' di Modena e Reggio Emilia)

Transparent conducting oxides (TCOs) are electrical conductive materials with a low absorption of light in the visible range. The unique combination of metallicity and transparency makes TCOs appealing for a variety of applications, including photovoltaic cells, flat displays, invisible electronics and plasmonics. TCOs are obtained by doping wide band-gap semiconductors with metal ions. Yet, the remarkable combination of conductivity in an albeit wide-gap (i.e., transparent) material is not fully understood, along with the effect of dopants on charge transport.

This work is focused on the atomistic understanding of the structural and optoelectronic properties of M-doped (M=Al, Ga, In) ZnO TCOs, which are indium-free, low-cost, and easy processable material, alternative to the standard Sn-doped  $\text{In}_2\text{O}_3$  (ITO). By using



first principles approaches, based on density functional theory, we first investigate how doping and defects affects the electronic properties of M-doped ZnO (MZO) up to the experimental solubility limit (3%–4%) [1-3].

As heavily doped semiconductors can exhibit a small negative real permittivity (i.e. high conductivity) and very small losses at the infrared and longer wavelengths, TCOs have been also proposed as plasmonic materials. We investigated the origin of near-infrared plasmonic activity in M-doped ZnO (MZO) transparent conducting oxides and we provide a microscopic insight on the formation of surface-plasmon polaritons at the Al:ZnO/ZnO interfaces in terms of characteristic lengths that can be measured by experiments. [4]

Finally we investigated the optoelectronic and thermoelectrical properties of MZO nanowires [5]. We show that the wires behave as 1D TCOs and low-loss plasmonic elements in the near IR and visible range. At the same time, the thermoelectric figure of merit results to be strongly enhanced upon nanostructuring with respect to ZnO bulk. We discuss the possibility to develop nanostructured energy converters in the form plasmon-heater/thermoelectric generator fully based on MZO nanowires.

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### #470 - Si-based TFT for biosensor applications: simulations and experimental results

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Micro-biosensors fabricated on Si-based technology could provide several advantages with respect to traditional technologies: small size and weight, fast response, device's analytical performance improvement and accuracy of the analysis, high reliability, lower energy consumption, possibility of packaging, on-chip integration of biosensors' arrays with the perspective of portable microanalysis systems, at low cost [1]. The two transduction mechanisms most used for biosensors are optical (indirect method) [2] and electrical (direct method) [3]. The last seems to provide several advantages in view of simple, portable and inexpensive detection devices.

In this work, we studied and verified the possibility to detect, through electrical transduction, hybridization of DNA molecules on MOS-like and thin film transistors (TFT). The devices were electrically characterized after the various stages of the functionalization process, consisting of oxide cleaning and activation; silanization; deposition and immobilization of biological molecules in localized region of sample (anchoring of oligonucleotide-DNA) [4].

The experimental results were compared with device simulations performed using a commercial software, Sentaurus®. We analyzed the structure by varying the fabrication parameters: body doping concentration, channel length, the thickness and the amount of charge on the sensitive "area" interface. For each structure, we simulated the electrical characteristics: capacitance vs voltage (CV), for transistors also the characteristic ( $I_d V_d$ ) and the transcharacteristic ( $I_d V_g$ ).

MOS-like devices vary their potential because of a detection event at the insulator/electrolyte interface. It is measured as a change in the capacitance due to immobilization of biological molecules or hybridization of a molecule of ssDNA with its complementary [3]. We experimentally found shift of 0.60 V due to DNA hybridization. The comparison with simulations demonstrated the ability to determine a priori DNA probe density of our devices in order to maximize their response.

We also explored the possibility of using a thin film transistor as a device for the detection of DNA hybridization recognition. We simulated different transistor structures and defined the best fabrication parameters. According to simulations, with  $2 \times 10^{12}$  electrons/cm<sup>2</sup> in the sensitive interface, a transcharacteristic shift of 1 V was obtained. Experimental measurements are in progress to verify the simulation results.

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### #471 - Photoinduced transient polarity at LaAlO3/SrTiO3 interfaces probed by time-resolved surface second harmonic generation

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*Other Authors: Andrea Rubano (Università Federico II), Tim Günter (University of Bonn), Manfred Fiebig (ETH Zurich), Fabio Miletto Granozio (CNR-SPIN), Lorenzo Marrucci (Università Federico II)*

Synthesis and device fabrication by interfacing different oxide materials have recently attracted a large attention because their physical properties can be easily tuned [1]. Among many interesting effects, the discovery of a high-mobility 2-dimensional electron gas (2DEG) at the interface between  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$  (LAO/STO), two insulating perovskites, is perhaps one of the most fascinating recent examples of interface-related phenomena. The 2DEG formation is a threshold process: for  $n \geq 4$  monolayers of LAO on STO the interface becomes metallic and even superconducting, and the insulator-to-metal (ITM) transition can be reversibly induced by an external electric field in the  $n = 3$  samples. An ITM transition may be induced by light irradiation too [2]. The latter phenomenon has recently attracted a considerable interest in view of potential optoelectronics applications and as a possible tool to investigate the fundamental physics of the system. So far all the studies focussed on the very slow response of photoconductivity, while, in general, the knowledge of the ultrafast processes governing the carrier relaxation in multilayer semiconductor structures is essential for designing high-speed electronic devices. However, despite their importance, the studies on LAO/STO that apply pump-probe techniques with fast temporal resolution, are still rare.

Here, by applying pump-probe surface second harmonic generation (SHG), we investigate the fast photoinduced mechanisms responsible of a transient build-up and depletion of the polarity at the LAO/STO interface. Compared to other standard optical techniques, SHG is extremely surface specific and, in the last decade, has emerged as a powerful tool for investigating polar-nonpolar oxide interfaces [3-5].

We have identified three basic microscopic processes, whose interplay leads to a complex dynamics of the transient interfacial polarity. First, an initial ultrafast diffusion of electrons sets up both a screening and a photo-Dember-induced electric field, that compete in opposition for modifying the interfacial polarity. Second, on a time-scale of hundreds of picoseconds, a transient polarity emerges because of the trapping of holes at the interface. The latter process is mediated by surface defective pinning centers. We find that the presence of  $\text{LaAlO}_3$  strongly influences the interfacial polarity dynamics by varying the relative strength of these three contributions.

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#### #472 - Monitoring and optimization of energy consumption of base transceiver stations

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The growth and development of the mobile phone network has led to an increased demand for energy by the telecommunications sector, with a noticeable impact on the environment.

Monitoring of energy consumption is a great tool for understanding how to better manage this consumption and find the best strategy to adopt in order to maximize reduction of unnecessary usage of electricity. This paper reports on a monitoring campaign performed on six BSs (Base Transceiver Stations) located central Italy, with different technology, typology and technical characteristics. The study focuses on monitoring energy consumption and environmental parameters (temperature, noise, and global radiation), linking energy consumption with the load of telephone traffic and with the air conditioning functions used to cool the transmission equipment. Moreover, using experimental data collected, it is shown, with a Monte Carlo simulation based on power saving features, how the BS monitored could save energy

#### #473 - CT-DSMC calculation of Oxygen transport properties on a non-vibrating O<sub>4</sub> PES

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Dilute molecular Oxygen flows are studied by modeling binary collisions, in the rigid rotor approximation, through an accurate Potential Energy Surface (PES) for the  $\text{O}_4$  dimer, obtained from molecular beams scattering experiments [1]. The PES accuracy is assessed by calculating molecular Oxygen transport properties (shear and bulk viscosity, self diffusion, thermal conductivity) by different equilibrium and non-equilibrium CT-DSMC based simulations that provide close values for the transport coefficients. Comparisons with available experimental data are presented and discussed in the temperature range 300-900 K, where vibrational degrees of freedom are expected to play a limited (but not always negligible) role. A sensitivity analysis is performed to study the impact of the PES uncertainties on the calculated transport coefficients.

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# October 2

<b>Advanced Microscopy Techniques</b>	<b>Roberto Pini</b>
<b>Out of Equilibrium Statistical Mechanics I</b>	<b>Bernardo Spagnolo</b>
<b>Econophysics</b>	<b>Rosario Mantegna</b>
<b>Environmental Physics and Pollution</b>	<b>WolfgangPlastino</b>
<b>Dosimetry</b>	<b>Maurizio Marrale</b>
<b>Quantum thermodynamics and quantum technologies 2</b>	<b>Fabio Taddei</b>
<b>Diamond-based substrates and Memristors for Brain sensing</b>	<b>Emilio Carbone</b>
<b>Metrology</b>	<b>Gianluca Galzerano</b>
<b>Fiber and Miniaturized Optical Sensors</b>	<b>Guido Toci</b>
<b>Electronical and optical properties of low dimensional systems III</b>	<b>Franco Gelardi</b>
<b>Synchrotron radiation and material science I</b>	<b>Carlo Mariani</b>
<b>Advanced materials for energy applications III</b>	<b>Giuliana Aquilanti</b>
<b>Molecular Biophysics II</b>	<b>Pierluigi San Biagio</b>
<b>Out of Equilibrium Statistical Mechanics II</b>	<b>Andrea Gambassi</b>
<b>Complex Networks in Economy, Biology, ...</b>	<b>Salvatore Miccichè</b>
<b>Physical Processes in Volcanic Eruptions</b>	<b>Costanza Bonadonna</b>
<b>Biomedical Applications</b>	<b>Maurizio Marrale</b>
<b>Complexity in the brain</b>	<b>Lucilla de Arcangelis</b>
<b>Nanomaterials and Nanotechnology: Graphene</b>	<b>Silvano Lizzit</b>
<b>Advanced optical characterization techniques</b>	<b>Gianluca Gagliardi</b>
<b>Synchrotron radiation and material science II</b>	<b>Federico Boscherini</b>

**#474 - High-resolution and high-speed optical manipulation of single biological molecules**

Marco Capitanio (I) - LENS - European Laboratory for Non-linear Spectroscopy

Other Authors: Francesco Pavone LENS - European Laboratory for Non-linear Spectroscopy

Force plays a fundamental role in a wide array of biological processes, regulating, for example, enzymatic activity, kinetics of molecular bonds, and molecular motors mechanics. Single molecule force spectroscopy techniques have enabled the investigation of such processes, but they are inadequate to probe short-lived (millisecond and sub-millisecond) molecular complexes. Such weak molecular interactions precede the formation of strong bonds and play an essential role in many biological processes. We developed a constant-force laser trap that allows us to investigate molecular interactions and sub-nanometer conformational changes occurring on a time scale of few tens of microseconds. [Capitanio *et al.*, *Nature Methods* 9, 1013-1019 (2012)]. The method is effective in studying the sequence-dependent affinity of DNA-binding proteins along a single DNA molecule. The improvement in time resolution provides important means of investigation on the long-puzzled mechanism of target search on DNA. In fact, one poorly understood issue in the field of protein-DNA interaction is how proteins weakly interact with non-cognate DNA sequences and how they efficiently find the sequence of interest among an extremely large amount of non-specific sequences. Using our technique, we could discriminate between two kinetically well-distinct populations of interactions between Lac repressor protein (LacI) and DNA, which clearly represent strong interactions with the specific (operator) sequences, and fast scanning of LacI along non-cognate DNA. We also demonstrate the validity of the method for the investigation of molecular motors' dynamics. We revealed a complex mechanism of regulation of myosin working stroke by force and previously undetectable fast detachment pathways. Our technique could be applied to a wide variety of non-processive molecular motors, single domains of processive motors, protein-DNA and protein-RNA interactions, and conceivably to any short-lived protein-protein interaction, opening new avenues for investigating the effects of forces on biological processes.

**#475 - Acoustic Force Spectroscopy**

Gijs Wuite (I) - VU University Amsterdam

With Acoustic Force Spectroscopy (AFS) we extend the force-spectroscopy toolbox with an acoustic manipulation device that allows exerting acoustic forces on many tethered molecules. AFS is a Lab-on-a-chip device consisting of a flow cell of two glass plates with a fluid chamber in between and a piezo element glued on top. While applying an alternating voltage to the piezo element, forces from sub-pN to hundreds of pNs are exerted to thousands of biomolecules in parallel, with sub-millisecond response time and inherent stability. We performed force-extension measurements on various DNA-protein interactions. These experiments demonstrate that AFS can be used to apply highly controlled forces up to at least 120 pN, with a force ramp speed between  $10^4$  –  $10^2$  pN/s and showing inherent stability over tens of hours over an observation area of at least  $1 \text{ mm}^2$ . Moreover, we demonstrate the use of AFS by mapping the energy landscape of the DIG/anti-DIG antibody-antigen bond over 6 orders of magnitude of force loading rates within several hours of experimentation. AFS distinguishes itself by its relative simplicity, low cost and compactness, which allow straightforward implementation in lab-on-a-chip devices. These aspects will help to spread single-molecule methods from the realm of fundamental research in specialized laboratories towards more wide-spread applications in for example molecular biology and medical diagnostics.

**#476 - 3D characterization at the nanoscale by stereoscopic scanning electron microscopy**

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Scanning Electron Microscopy (SEM) is a 2D microscopy technique, providing information related to morphology, composition and other properties of bulky samples. We discuss the access to 3D characterization down to the nanoscale based on stereoscopy, a technique already well assessed on the macroscopic scale. In the simplest case, as in the human vision, at least a couple of stereo images are acquired at different inclination. The relative displacement of a feature in the different images allows to determine its elevation with respect to a reference plane. In this work, the process was tested on images showing details at the scale of tens of nm. The position of sparse points at sample surface was reconstructed according to several approaches. First, the features in the two images were directly recognized and matched by the operator, in order to maintain the highest degree of control on the process. A 3D positional uncertainty lower than 14 nm was obtained for small nanostructures lying on regular surfaces, evaluated in excess as the standard deviation of the set of reconstructed positions from the geometrical reference surface. The main limiting factors for the 3D reconstruction result to be the limited amount of uniquely recognizable features, the ratio between field of view and resolution and the contrast attainable at high magnification. As a second step, several strategies for the automatic feature recognition on each image and for their matching between different image projections were tested. The most promising algorithm proved to be the so called Speeded Up Robust Features local detector and descriptor. A rather conservative set of parameters was

used in order to limit the results only to reliably matched features. The algorithm proved to be able to position the nanostructure center of mass with a reliability of the order of 2 nm, comparable to lateral resolution of the SEM images. The automatic approach could result in a reduction, by several order of magnitudes, of the number of matched features with respect to the direct operator recognition, depending on the choice of parameters and filters. Nevertheless, the 3D standard deviation from the reference geometrical surface found in this case was estimated lower than 12 nm. Fully automatic reconstruction may be a reliable option only when the feature contrast is outstanding and their distribution dense. Similar reconstructions were done on dense distributions of 50 nm sized structures on silver ink drops deposited on spin coated polymer substrates. These show rougher surfaces where a standard deviation of 18 nm from the reference geometrical surface was obtained.

#### #477 - Advanced TEM characterizations of CuO Nw for water purification

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Environmental safety is one of the serious concerns for the humanity because of rapid increase in the use of organic pollutants in agriculture and industries which cause severe adverse effects on the environment. In this contest, copper oxide is a promising candidate for wastewater treatment. In fact it has received much attention as a photocatalyst large band gap material.

Indeed, cupric oxide (CuO) and cuprous oxide (Cu<sub>2</sub>O) are *p*-type metal oxide semiconductor with a band gap of 1.3 eV and 2.2 eV, respectively.

In this work, we synthesized CuO nanowires by a thermal process in oxygen ambient of a Cu foil. Nanowires were morphologically and structurally characterized by scanning and transmission electron microscopy (SEM and TEM), energy dispersive X-ray (EDX) analysis and X-ray diffraction. The material shows a high density of CuO nanowires, more than 10 microns in length and ~50 nm in mean diameter. A subsequent thermal annealing induced a controllable stoichiometry transformation of both the nanowires and the underlying substrate, from the CuO to Cu<sub>2</sub>O phase. As a further investigation, we performed an in-situ thermal treatment inside the TEM for a better understanding of the CuO to the Cu<sub>2</sub>O transition. High-resolution TEM and diffraction analyses on single nanowire were performed in order to evaluate the morphology and the crystallinity of the wires before and after the annealing. As a further experiment we analyzed single CuO nanowire by scanning TEM and STEM, in order to obtain a local chemical characterization. The synthesized materials were tested towards the degradation of organic compounds in water showing a better photocatalytic action of CuO nanowires related to their lower defectivity with respect the Cu<sub>2</sub>O ones.

#### #478 - EFFECTS OF CELL PROLIFERATION INHIBITORS INVESTIGATED BY DELAYED LUMINESCENCE SPECTROSCOPY

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The possibility of using phot-induced Delayed Luminescence (DL) of living cells to monitor the effects of some cancer treatment that inhibit cell proliferation and induce apoptosis has been investigated. Different human cancer cell lines were investigated and DL measurements from liquid suspension of cultured cells, in the time interval 10  $\mu$ s – 1 ms after the switching off of the illumination source, were performed on treated samples and compared to untreated ones. In particular the time decay of two spectral components, the blue (emission wavelength 460 nm) and the red components (emission wavelength 645 nm) were analyzed.

The obtained data showed to be consistent with an important role of the Mitochondrial Respiratory Chain in DL emission. Changes in DL parameters can be correlated to apoptosis level. In particular changes in the DL blue component (connected to the mitochondrial level of nicotinamide adenine dinucleotide, NADH) may be a hallmark of induced apoptosis, while the response in the red spectral range may be ascribed to oxygen effects, as or Protoporphyrin IX emission quenching (that could be correlated to iron homeostasis in the cell) or dimol photoemission generated by two colliding molecules of singlet oxygen charge (that could be correlated to recombination in Fe/S redox centers in Complex I).

#### #479 - Stimulated Raman scattering in between nano and biophotonics applications

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Nonlinear optics at nanoscale is a recent fascinating research field of great importance. Among the numerous nonlinear optics phenomena, due to its significant implications from both fundamental and applicative point of view, stimulated Raman scattering is one of the most interesting. Concerning the SRS fundamental point of view, there have been a number of investigations both experimental and theoretical, but the question is still "open". From an applicative point of view, Raman amplification, demonstrated in the early 1970s, is an interesting approach for optical amplification, because it is only restricted by the pump

wavelength and Raman active modes of the gain medium. Concerning SRS at nanoscale there are some important prospective, for example to realize micro/nano source, with improved performances, based on SRS. Nanostructured silicon has generated large interest in the past decades as a promising key material to establish a Si-based photonics. We report the first observation of stimulated Raman scattering in silicon nanocrystals embedded in a silica matrix under non-resonant excitation at infrared wavelengths. Raman gain is directly measured as a function of the silicon content. A giant Raman gain from the silicon nanocrystals is obtained that is up to four orders of magnitude greater than in crystalline silicon.

In life science, Raman microscopy can be used as contrast mechanism based on vibrational properties. A typical Raman spectrum makes available information on the molecular and chemical structure of the sample, thereby offering an intrinsic chemical selectivity. However, linear Raman microscopy is limited to weak signals, so, to obtain an image, acquisition times are very long, generally varying between 1ms to 1s per pixel. A multiphoton microscopy based on Coherent-Raman Scattering was studied as an alternative way to provide vibrational contrast. The Raman signal, generated by the non-linear interaction among pump and probe signals and the sample, is much more intense respect to linear Raman microscopy, being coherent and propagating along the axis of oscillating molecules. Thus, the acquisition times are considerably reduced allowing, in principle, the acquisition of images on a large area in a few seconds. This technique presents the advantage to be completely label-free, with the ability to have an excellent signal-to-noise ratio that occurs in an image obtained in a few seconds and with a good image contrast. We report femtosecond stimulated Raman spectroscopic and microscopy implementation. As a preliminary step for nonlinear microscopy, label free imaging of polystyrene-beads is demonstrated.

#### #480 - Dip Pen Lithography of oligonucleotides on flexible substrates for point-of-care malaria disease testing

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The first step for prevention and treatment of diseases is the accurate diagnosis. However, proper diagnostic technologies are not available in developing countries due to the lack of reliable electrical power, refrigeration and trained personnel. For this reason, there is an urgent need of low cost, rapid assays not requiring any external support. By coupling such technologies to communication infrastructures, healthcare in areas without access to medical personnel would be possible. "Paper" like substrates are ideal for fabricating such devices since they are cheap, easy to degradate after use and compatible with most of existing printing technologies [1]. We had previously shown the possibility to efficiently deposit oligonucleotides by Dip Pen Lithography(DPL) onto glass surfaces [2]. In this work, we deposited oligonucleotides on nylon substrate for the fabrication of biochips usable for detecting the activity of human topoisomerase I. Subsequently, the chip will be modified to detect the Malaria-causing *Plasmodium* parasites through the detection of *Plasmodium* topoisomerase I activity [3]. We optimized oligonucleotides printing on nylon substrate, obtaining efficient deposition at 10 - 1 uM oligonucleotide concentrations, 70% relative humidity and 30% glycerol v/v. We obtained circular spots with diameter in the range of 30 - 50 microns, with the dimension being a function of dwell time (1s - 20 s). DPL operation needs ultra tiny amounts of DNA (as low as 0.5 uL, 10 - 1 uM concentration) for printing thousands of spots in a single run so reducing material consumption in comparison with standard bioprinting techniques [4]. In a first set of experiments, the printed oligonucleotides was hybridized with a fluorescence-labelled complementary probe to detect and quantify DNA after DPL deposition. In subsequent experiment, the spotted oligonucleotides generate a topoisomerase substrate, which upon reaction with the enzyme will be coupled to a fluorescently labelled oligonucleotide to allow detection of a signal. In conclusion, the combination of DPL and topoisomerase detection onto nylon substrates would be a suitable solution for point-of-care diagnostic chips fabrication.

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**#481 - Nonlinear relaxation phenomena in three different systems of condensed matter***Bernardo Spagnolo (I) - Università di Palermo**Other Authors: Davide Valenti, Dominique Persano Adorno, Claudio Guarcello, Luca Magazzù, Angelo Carollo Dipartimento di Fisica e Chimica, Group of Interdisciplinary Theoretical Physics, Università di Palermo and CNISM, Unità di Palermo, Viale delle Scienze, Edificio 18, I-90128 Palermo, Italy*

Nonlinear relaxation phenomena in three different systems of condensed matter are investigated. (i) First, the phase dynamics in Josephson junctions is analyzed. Specifically, a superconductor-graphene-superconductor (SGS) system exhibits quantum metastable states, and the average escape time from these metastable states in the presence of Gaussian and correlated fluctuations is calculated, varying the noise source intensity and the bias frequency. Moreover the transient dynamics of a long-overlap Josephson junction (JJ) subject to thermal fluctuations and non-Gaussian noise sources, Lévy type, is investigated. Noise induced phenomena are observed, such as the noise enhanced stability and the resonant activation. The analysis of the time evolution of the order parameter highlights the influence of the noise induced solitons on the mean switching time behavior and the observation of breathers. (ii) Second, the electron spin relaxation process in n-type GaAs crystals driven by a fluctuating electric field and two different noise sources is investigated. Monte Carlo numerical simulations show, in both cases, an enhancement of the spin relaxation time by increasing the amplitude of the external noise. (iii) Finally, the stabilization of quantum metastable states by dissipation is presented. Normally, quantum fluctuations enhance the escape from metastable states in the presence of dissipation. We show that dissipation can enhance the stability of a quantum metastable system, consisting of a particle moving in a strongly asymmetric double well potential, interacting with a thermal bath. We find that the escape time from the metastable region has a nonmonotonic behavior versus the system-bath coupling and the temperature, producing a stabilizing effect.

**#482 - Kondo effect in carbon nanotubes***Milena Grifoni (I) - University of Regensburg*

The Kondo effect is an archetypical manifestation of strong electronic correlations in mesoscopic systems. A degeneracy of quantum states required for its occurrence is usually provided by the electronic spin degree of freedom, resulting in the so-called SU(2) Kondo behavior. Remarkably, in the Kondo regime the differential conductance obeys universal scaling as a function of temperature, bias voltage, and magnetic field.

Clean carbon nanotubes (CNTs) provide a unique test-bed for the investigation and manipulation of the quantum dot level structure and its consequences for the Kondo effect. In CNTs an additional degeneracy in the intrinsic low energy spectrum stems from the sublattice symmetry of the graphene lattice, and enables one to study unconventional correlation phenomena such as the spin plus orbital SU(4) Kondo effect.

The sublattice symmetry, though, is broken by a finite spin-orbit coupling or by a boundary induced valley mixing, and is visible in the presence of satellite Kondo peaks in the nonlinear transport.

Strikingly, experiments studying the evolution of the central Kondo peak and of its satellites in magnetic fields applied parallel and perpendicular to the tube's axis, reveal selection rules in the inelastic virtual processes contributing to the Kondo resonance. We discuss the origin of these selection rules. Additionally, we present a

novel approach to the non-equilibrium Kondo problem, based on the Keldysh effective action, which well reproduces the rich experimental observations.

**#483 - Decoherence-induced topological phase transition in 1D fermion model.***Angelo Carollo - Palermo**Other Authors: Fabio Anzà, Davide Valenti, Bernardo Spagnolo*

We explore decoherence-induced topological phase transitions of fermions in 1D lattice in the non-equilibrium steady state of an open system with local reservoirs. In particular we focus on a spin-full version of the so called 1D Kitaev chain and consider the effect of quasi-local decoherence and dephasing as a tool to induce non-trivial topological phases. The 1D Kitaev chain is a prototypical example of a system which shows topological order, signalled by the presence of an odd number of spatially separated Majorana zero modes. Depending on the Hamiltonian parameters, such a system undergoes a transition from a topologically trivial to a non-trivial phase. We show that a suitably engineered decoherence may indeed enact a similar transition to a topologically non-trivial phase, starting from an otherwise trivial one. Such a phenomenon is the result of the interplay between Hamiltonian and dissipative interactions. These findings are relevant for applications in solid state physics as well as in the context of cold-atoms.

**#484 - On-demand recovery of hidden entanglement by local operations within non-Markovian dynamics***Giuseppe Falci - Università di Catania**Other Authors: Antonio D'Arrigo (University of Catania), Adeline Orioux (University of Roma, La Sapienza), Giacomo Ferranti (University of Roma, La Sapienza), Giuliano Benenti (Insubria University, Como), Elisabetta Paladino (University of Catania), Rosario Lo Franco, (University of Nottingham), Fabio Sciarrino (University of Roma, La Sapienza), Paolo Mataloni (University of Roma, La Sapienza)*



In many applications entanglement must be distributed through noisy communication channels that unavoidably degrade it. Entanglement cannot be generated by local operations and classical communication (LOCC), implying that once it has been distributed it is not possible to recreate it by LOCC. Recovery of entanglement by purely local control is however not forbidden in the presence of non-Markovian dynamics. We investigate the phenomenon of bipartite entanglement revivals under LOCC in systems subject to local and independent classical noise sources, explaining this apparent paradox by introducing the concept of "hidden" entanglement, the amount of entanglement that cannot be exploited due to the lack of classical information on the system. We show and demonstrate in two all-optical experiments that such entanglement can be restored on-demand. First, we implement an open-loop control scheme based on a purely local operation, without acquiring any information on the environment; then, we use a closed-loop scheme in which the environment is measured, the outcome controlling the local operations on the system. Relying on local control, both schemes improve the efficiency of entanglement sharing in distributed quantum networks.

#### #485 - Information-theoretic zeroth law

*Fabio Anza - Atomic & Laser Physics Department, Oxford University*

*Other Authors: Vlatko Vedral (Oxford University)*

An analogy between the dynamical behavior of a classical and a quantum gas in a box is considered. Building the intuition on that, I propose a new notion of equilibrium for a quantum system in a pure state, inspired by the zeroth law of thermodynamics and by Jaynes' work on statistical mechanics. Arguing that the relevant notion is Shannon's entropy, the characterization of the equilibrium distribution is given in term of two equations. Simple applications of the posited notion of equilibrium are considered and the relation of such an approach with both ordinary quantum statistical mechanics and recent approaches to thermalization of closed quantum systems are discussed.

#### #486 - Synthesizing Quantum States in Ultrastrong Optomechanics

*Vincenzo Macrì - Università degli Studi di Messina*

*Other Authors: L. Garziano, R. Stassi, S. Savasta, and O. Di Stefano, Università degli Studi di Messina*

We describe how ultrastrong interactions in cavity-optomechanics can be exploited to force the ground state of the optomechanical system to evolve into an arbitrary quantum state of mechanical motion in a completely controlled and deterministic manner [1]. If the target quantum state is a superposition of  $N$  Fock states, it can be obtained by applying in single-step  $N$  classical optical signals of different frequencies for a common time interval. This protocol can be applied to various strongly interacting quantum systems as trapped ions beyond the Lamb-Dicke regime and cavity QED into the ultrastrong coupling regime [2]. We further extend this scheme to generate mechanical NOON states with large phonon numbers in a deterministic way or with high probability.

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#### #487 - Josephson Junctions response to stochastic and periodic perturbations for signal detection

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We investigate the possibility of exploiting the speed and low noise features of Josephson junctions for detecting sinusoidal signals corrupted by Gaussian noise. In particular we discuss how to exploit the occurrence of stochastic resonance [1] in Josephson junctions with the methods of signal processing [2]. Josephson junctions are very sensitive to a small periodic signal embedded in the noise, and therefore the escape times from the locked state can be employed to reveal the presence of the sinusoidal component [3,4]. The loss of information that occurs retaining only the sequence of escapes, rather than the full trajectory, is mild if optimal signal processing strategies are applied. The proposed detection scheme, in the framework of statistical decision theory (Neyman-Pearson) shows some remarkable features, such as quasi-optimal scaling behavior and stochastic activation. The analysis of the escape times is generic for metastable potentials. It can therefore be extended to other systems, such as a quasi-Hamiltonian pendular Fabry-Perot interferometer [5]. Placed inside one of the minimum of the optomechanical potential an escape can be revealed by the sudden change of reflectivity near the top of the potential well.

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#### #488 - Adiabatic manipulation of architectures of multilevel artificial atoms.

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The ability of manipulating multilevel coherence in solid-state "artificial atoms" architectures would be a key issue for several achievements both in fundamental and in applied physics. In this contribution we address the implementation of a Lambda scheme in superconducting  $N > 2$  "artificial atoms" which is a fundamental building block of such architectures, and study coherent population transfer (CPT) as a benchmark process for quantum control.

Introduce two new protocols to implement quantum state engineering by population transfer in solid-state Circuit-QED or nanoelectromechanical architectures. The first is a 2+1-photon scheme allowing for a Lambda configuration at the symmetry point, which minimizes noise, despite of selection rules, and can be applied to present technology high-quality superconducting qubits. The second is a protocol where CPT is obtained with the constraint of an always on field, mimicking an unswitchable hardware coupling.

We finally address the problem of detecting signature of the ultrastrong coupling in atom-cavity systems. We show that a new channel for CPT is opened, whose detection is a "smoking gun" for the existence in Nature of this new ultrastrong regime of coherent coupling with the electromagnetic field. We show how a ~100% efficiency of detection can be achieved in systems of many artificial atoms strongly coupled to a cavity, fabricable within present technology.

#### #489 - Quantum quench within the gapless phase of the XXZ spin-chain

*Mario Collura - SISSA, Statistical Physics*

We consider the nonequilibrium unitary dynamics induced by suddenly switching on the interactions in the XXZ spin-1/2 chain. Although the model is integrable, and much effort has been spent in order to understand some of its equilibrium properties, still very little is known both for the exact time evolution and the stationary values of local observables after a quench, especially in the gapless phase. Anyhow, in thermodynamic equilibrium, the low-energy properties of the XXZ spin chain in the gapless phase are well described by the Luttinger model as it can be derived by bosonization of the spin chain Hamiltonian. Obviously, this effective low-energy description is expected to fail for the description of the quench dynamics since in changing a Hamiltonian parameter for a finite value, an extensive amount of energy is pumped into the system resulting in the population of eigenstates of the post-quench Hamiltonian which are not described by the Luttinger liquid approximation. However, it is still natural to wonder whether the simple results obtained for the quantum quench in the Luttinger model can effectively describe the non-equilibrium dynamics of the spin chain, at least in some parameter regimes and/or specific time windows. We address this question by solving the dynamics of the XXZ model by means of extensive iTEBD (infinite time-evolving block decimation) simulations. In particular, for spin-spin correlation functions we find a surprising agreement between exact numerical results and Luttinger model description.

**#490 - Systemic risk and early-warning signals in financial networks**

*Diego Garlaschelli (I) - Lorentz Institute for Theoretical Physics, University of Leiden*

The global financial crisis shifted the interest from traditional measures of "risk" of individual banks to new measures of "systemic risk", defined as the risk of collapse of an entire interbank system. Estimating systemic risk requires the knowledge of the whole network of exposures among banks. However, due to confidentiality issues, banks only disclose their total exposure towards the aggregate of all other banks, rather than their individual exposures towards each bank. Is it possible to statistically reconstruct the hidden structure of a network in such a way that privacy is protected, but at the same time higher-order properties are correctly predicted? In this talk, I will present general network reconstruction methods and discuss their remarkable performance on various economic, social, and biological systems, with an emphasis on interbank networks. Then, as a counter-example, I will show an analysis of the Dutch interbank network performed in collaboration with the Dutch Central Bank. We found that many standard topological properties of this network (such as the number of pairs of banks with mutual connections) display an abrupt change in 2008, providing a clear - but unpredictable - signature of the crisis. By contrast, after controlling for the heterogeneous connectivity of banks, the same properties show a gradual transition to the crisis, starting in 2005 and preceded by an even earlier period during which anomalous debt loops could have led to the underestimation of counter-party risk. Unlike in the other examples discussed in the talk, these deviations from the reconstructed ensemble are significant and can be used as early-warning signals of the upcoming crisis. By definition, these early warnings are undetectable if the network is reconstructed from partial bank-specific data. We discuss important implications for network modelling and bank regulatory policies.

**#491 - Exactly-solvable non-Markovian dynamic network**

*Enrico Scalas (I) - Department of Mathematics, University of Sussex*

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Non-Markovian processes are widespread in natural and human-made systems, yet explicit modelling and analysis of such systems is underdeveloped. In this letter we consider a dynamic network with random link activation and deletion (RLAD) with non-exponential inter-event times. We study a semi-Markov random process when the inter-event times are heavy tailed Mittag-Leffler distributed, thus considerably slowing down the corresponding Markovian dynamics and study the system far from equilibrium. We derive an analytically and computationally tractable system of forward equations utilizing the Caputo derivative for the probability of having a given number of active links in the network.

**#492 - Bank's centrality and interbank market funding rates**

*Giulia Iori - City University London*

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This paper empirically investigates the role of the position of a bank on the interbank market on its funding rates. Specifically we analyse transaction data from the e-MID market, which is the only electronic interbank market in the Euro Area and US, over a period 2006–2009, that encompass the global financial crisis. We show that interbank spreads are significantly affected by both, local and global, connectedness measures. Overall we find that lenders pay a premium for being more central. Borrowers, on the other hand, pay a premium (i.e. pay higher rates) for maintaining better local connectivity, but receive a significant discount for achieving global higher centrality.

**#493 - Designing guarantee options in defined contribution pension plans**

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The shift from defined benefit (DB) to defined contribution (DC) is pervasive among pension funds, due to demographic changes and macroeconomic pressures. In DB all risks are borne by the provider, while in plain vanilla DC all risks are borne by the beneficiary. For DC to provide income security some kind of guarantee is required. A minimum guarantee clause can be modeled as a put option written on some underlying *reference portfolio* of assets and we develop a discrete model that optimally selects the reference portfolio to minimise the cost of a guarantee. While the relation DB-DC is typically viewed as a binary one, the model can be used to price a wide range of guarantees creating a continuum between DB and DC. Integrating guarantee pricing with asset allocation decision is useful to both pension fund managers and regulators. The former are given a yardstick to assess if a given asset portfolio is fit-for-purpose; the latter can assess differences of specific reference funds with respect to the optimal one, signalling possible cases of moral hazard.

We develop a general and computationally tractable model for pricing the cost of alternative embedded guarantee options in DC pension funds. The model determines the asset allocation choice that is optimal for a given guarantee, in that it minimizes the cost of the guarantee. The model is tested using real-world data to illustrate the effect of the design parameters of the guarantee on the

cost of offering the option. Results illustrate the effect on the option of (i) level of guarantee, (ii) amount of equity, and (iii) participation of the beneficiaries in any portfolio upswing above the guarantee. We also show how the model can be used to benchmark existing portfolios by applying it to test portfolios of State and local government pension funds from the literature. Our results are in agreement with empirical findings of existing literature, but also attribute the precise cost of the guarantee. We also show how the model can be used to calculate risk premia for risk sharing. The model we implement and test can be extended to cover a broad range of guarantees that increasingly resemble DB, thus providing a continuum of funds in the hitherto dichotomous relation DC-DB. Some extensions are straightforward to build and calibrate, while others are provided as areas for further research.

Paper available at [http://papers.ssrn.com/sol3/papers.cfm?abstract\\_id=2563087](http://papers.ssrn.com/sol3/papers.cfm?abstract_id=2563087)

#### #494 - Systemic Risk and Macro-prudential policies: a credit network-based approach

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Assessing systemic risk and defining macro-prudential policies aiming at reducing economic system vulnerability have been at the center of the economic debate of the last years (Basel Committee, 2011; Yellen, 2011; Angelini et al., 2012). Credit networks play a crucial role in diffusing and amplifying local shocks, thus we try to define both early warning indicators of crises and policy precautionary measures based on the analysis of the dynamics of credit network connectivity (Delli Gatti et al., 2010; Battiston et al., 2012).

Following the network-based financial accelerator approach (Delli Gatti et al., 2005, 2010; Riccetti et al., 2013), we constructed an agent based model reproducing an artificial credit network populated by heterogeneous firms and banks. In the attempt of gaining satisficing levels of realized profits, firms and banks choose their target level of leverage through a simple reinforcement learning procedure (Tefsatson, 2005; Riccetti et al., 2013; Catullo et al., 2015). Thus, agents' choices about their target leverage determine individual and, thus, aggregate loan demand and supply, which in turn shape the evolution of the credit network, influencing aggregate output dynamics.

We calibrated the model on a sample of firms and banks quoted on Japanese stock-exchange markets from 1980 to 2012 (Marotta et al., 2013). The model simulations generate endogenous pro-cyclical fluctuations of credit and connectivity. Indeed, according to the methodology developed by Schularick and Taylor (2012), we found that both credit and connectivity growth rates are correlated with crisis probability and their combination represents an effective early warning measure in both empirical and simulated data, which thus may be used to define loan-to-value macro-prudential interventions.

Simulation experiments show that when systemic risk increases beyond a certain threshold, forcing banks to avoid lending to more indebted firms may decrease output volatility without causing consistent credit and, thus, output contractions. We tested also permanent loan-to-value restrictions targeted only to more connected banks. When interventions focus on banks that are relatively central in the credit network, economic system vulnerability may be substantially reduced without affecting aggregate credit supply and output. Concluding, the analysis of credit network connectivity may be useful for assessing system risk. Moreover, agent based models which endogenize credit and connectivity dynamics may be helpful for testing the effectiveness of early warning indicators and the results of macro-prudential policies.

#### #495 - Discovering SIFIs, a temporal complex approach

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This paper proposes an intrinsically temporal methodology to identify Systemically Important Financial Institutions (SIFIs) and to track their common activity over time. The introduction of the temporal dimension gives the opportunity to develop an early warning indicator for the risk associated to the whole network where the strength of contemporaneous spillover effects is summarized in a single variable: the time score.

Moreover, the same solution method can be used to identify the community structure of the network and the systemic importance of banks within each community, tracking their activity through time.

The technique is based on tensor decomposition, where a temporal network is naturally represented as a time-ordered sequence of adjacency matrices, each one describing the state of the ...financial network at a given point in time.

Our method is able to take into account both the spatial and the temporal distribution of the links that represent flows of funds between institutions.

We apply the method to the e-Mid dataset, the most central banks turn out to be Italian banks. The cross-correlation between the traded volume and the time score coefficient founded by the decomposition shows how this series anticipates the movement in the overall traded volume.

**#496 - Random Investments in Financial Markets**

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In this paper, we address the specific role of randomness in financial markets, both at micro and macro level. In particular, we will review some recent results obtained about the effectiveness of random strategies of investment, compared with some of the most used trading strategies for forecasting the behavior of real financial indexes [1,2]. We also push forward our analysis by means of a Self-Organized Criticality model, able to simulate financial avalanches in trading communities with different network topologies, where a Pareto-like power law behavior of wealth spontaneously emerges [3,4]. In this context we present new findings and suggestions for policies based on the effects that random strategies can have in terms of reduction of dangerous financial extreme events, i.e. bubbles and crashes.

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**#497 - Randomizing bipartite networks: the case of the World Trade Web**

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The class of networks represented by bipartite networks has been recognized to provide a particularly insightful representation of many different systems: ecological networks, trade networks, citations and collaboration networks represent only few examples. Anyway, quite surprisingly, little work has been done so far to implement null models on real bipartite networks. In particular, null models for bipartite networks proposed so far show several limitations, ranging from being purely numerical (thus lacking the analytic character), to assuming an a priori functional form either for the distribution of the quantities of interest or for the model's parameters (thus not being real data-rooted) or, lastly, using approximate analytical models. In this paper, we propose a theoretical framework guaranteeing the three aforementioned properties, extending a recently-proposed method to randomize monopartite networks to bipartite networks. The method rests upon the sequential maximization of Shannon entropy and the likelihood function, a combination which has been proven to be highly effective both for detecting patterns and to reconstruct the structure of several real-world networks. While the proposed formalism is perfectly general, in this paper we apply our method to the binary, undirected, bipartite representation of the World Trade Web, as described by two different data sets (1963-2000 and 1995-2010). We extend the definition of several monopartite quantities of interest to the bipartite case and compare the output of our null model with the observed trends. Such a comparison shows that the bipartite WTW behaves completely differently from the monopartite WTW. Remarkably, the bipartite definition of the closed motifs (here proposed for the first time), allows us to detect early-warning signals of the 2007-2008 crisis (dating back to 2003) witnessed by the increasing level of randomness of the observed network structure. Moreover, signals of the crisis attenuation after 2007 seem to be visible.

**#498 - Radioxenon Atmospheric Transport Modeling: from Worldwide Impact of Nuclear Power Plants to CTBTO event screening categorization**

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The International Monitoring System (IMS), which is currently built up by the Comprehensive Nuclear-Test-Ban Treaty Organization (CTBTO), continuously takes environmental measurements including atmospheric concentrations of several radionuclides. The characterization of the existing and legitimate background, which is produced mainly by Nuclear Power Plants (NPPs) and Isotope Production Facilities (IPFs), is of high interest to improve the capabilities of the monitoring network. Over 400 reactors at NPPs are currently in operation worldwide, while only five IPFs are considered to be continuously emitting relevant activity levels. Nevertheless, the emission strengths of typical nuclear power reactors are below the emission strengths of these IPFs; a typical IPF usually emits radioxenon in the order of magnitude or above the total of all operational NPPs together. Therefore, the long-term global radioxenon background is a result of many weak and a few strong sources.

The emissions from legitimate sources can usually only be estimated. However, historic source terms of  $^{133}\text{Xe}$  emissions from the IPF at ANSTO, Sydney (Australia), have been made available in a daily resolution, and then applied together with Atmospheric Transport Modelling (ATM) to predict the concentration time series at two radioxenon monitoring stations: Melbourne (Australia) and Chatham Island (New Zealand).

Moreover, following the Fukushima NPP accident, detections of  $^{133}\text{Xe}$  have been made in various locations. Using results of these remote measurements, the Fukushima  $^{133}\text{Xe}$  source term has been reconstructed and compared with previously estimated  $^{137}\text{Cs}$  and  $^{131}\text{I}$  source terms.

Finally, feedback induced by local meteorological patterns on the equipment and on the sampling procedures has been included in the analysis to improve CTBTO event screening categorisation. The occurrence probability of radioxenon outliers has been estimated with a time series approach characterising and avoiding the influence of local meteorological patterns.

**#499 - IMPACT OF ENVIRONMENT AND CLIMATE ON CULTURAL HERITAGE**

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Atmospheric and climate sciences have substantially contributed to scientific research applied to the protection of cultural heritage towards environmental impact. Relevant research results developed in this sector by national and international projects will be presented, concerning in particular the evaluation of air pollution and climate change impact on cultural assets, both indoor and outdoor located.

Despite the strong interest focused on these areas, both at research and policy levels, very little attention has so far been directed towards the impact of future change on cultural heritage: this is unacceptable either in Europe and in Italy being cultural heritage a non-renewable resource to be transmitted to future generations.

In order to fill this gap, an innovative research work has been realized within the Noah's Ark Project, funded by the European Commission, which produced, as results, the "Atlas of climate change impact on European Cultural Heritage".

The study performed included as initial step the identification of the most relevant climate parameters affecting cultural heritage (e.g. yearly precipitation, rainfall intensity) for producing climate maps. Subsequently, the parameters were combined to produce specific heritage climatologies, e.g. wet-frost, based on rain followed by intense freezing, allowing the preparation of the heritage climate maps. A further step employed climate parameters to determine the amount of damage occurring on building materials in future scenarios, and to obtain the damage maps (e.g. stone surface recession, metal corrosion). Finally risk maps were prepared combining two or more damage processes that could occur in different regions of Europe. Guidelines were also formulated in order to inform cultural heritage managers and stakeholders on the effects of climate change on built heritage. The presentation will summarize some of the results achieved.

As described, the Italian scientific community has played and is playing a leading role in this area of research.

In fact, recently, ISAC-CNR started a collaboration work to study the environmental impact in extra-Europe areas, in particular in Panama, Central America, where the climate change at that latitudes can have different effects on the monuments. This study will enhance the knowledge in facing extreme events and it will support the preservation of UNESCO sites located in this region. It will be also provided a synthetic picture of the activities in the field of training, technology transfer and the dissemination of knowledge among decision makers.

The presentation will conclude with a summary of the Joint Programming Initiative "Cultural Heritage and Climate Change: a new challenge" coordinate by Italy (i.e. Ministry of Education, University and Research-MIUR and Ministry of Cultural Heritage and Activities and Tourism- MIBACT) since 2010 with 18 EU Participating Countries.

**#500 - Early indicators of abrupt desertification transitions**

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Regime shifts in ecosystems can imply relevant economic and social effects. This is especially true when they involve abrupt transitions occurring on a relatively short timescale [1-4]. A special case of regime shift is given by desertification transitions of semi-arid ecosystems which can be strongly affected by climatic or anthropogenic factors [1,3]. A crucial issue in this field concerns the identification of early and reliable transition indicators, providing not only an estimate of the desertification risk, but also a tool to monitor the effectiveness of actions devoted to contrast it [1,3]. To this purpose, several new transition indicators have been proposed [3,4]. In particular, at increasing values of the mortality rate (control parameter of the transition) very early indicators have been recently identified in the case of continuous or nearly continuous transitions (where the order parameter of the transition is the fraction of vegetation covered surface). These new early indicators are associated with a change in the skewness sign of the fluctuation distribution of the size of both the biggest clusters: the vegetation covered and the non-vegetated one [4]. On the other hand, numerical simulations based on a stochastic cellular automaton model [5,6] showed that several physical and ecological parameters, like in particular the colonization rate and the aridity parameter, can affect the character of the transition: from continuous to abrupt or vice versa [6,7]. Here we discuss the possibility of extending the new indicators to the case of abrupt transitions. [1] J. F. Reynolds et al., *Science*, 316, 847 (2007). [2] K. M. Dahlin, G. P. Asner, C. B. Field, *Proc. Nat. Ac. of Science*, 110, 6895 (2013). [3] S. Kéfi, V. Guttal, W. A. Brock, S. R. Carpenter, A. M. Ellison, V. N. Livina, D. A. Seekell, M. Scheffer, E. H. van Nes, V. Dakos, *PLoS One*, 9, e92097 (2014). [4] R. Corrado, A. M. Cherubini, C. Pennetta, *Phys. Rev. E*, 90, 062705 (2014). [5] S. Kéfi, M. Rietkerk, C. L. Alados, Y. Pueyo, V. P. Papanastasis, A. ElAich, P. C. de Ruiter, *Nature*, 449, 213 (2007). [6] S. Kéfi, M. Rietkerk, M. van Baalen, M. Loreau, *Theor. Popul. Biology*, 71, 367 (2007). [7] R. Corrado, A. M. Cherubini, C. Pennetta, *Commun. Nonlinear Sci. and Numer. Simulat.* 22, 3 (2015).

#### **#501 - A fully automated Raman lidar: measurements of the atmospheric aerosol optical transmission and water vapour vertical profiles at service of Ultra High Energy Cosmic Ray (UHECR) Observatory P. Auger.**

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A robust and low cost Raman lidar is installed in the center of the P. Auger Observatory (AUGER), it is designed to measure the aerosol extinction and backscatter coefficients, as well as the vertical profiles of the water vapour mixing ratio. This system is taking measurements almost continuously, and in full automatic mode since November 2013. We report examples of observations to discuss the performances of this Raman lidar in producing the vertical aerosol optical depth profiles for the needs of the AUGER Observatory, and its capabilities to constitute a feasible and useful database for atmospheric studies related to the climatology of aerosol optical properties and of water vapour in planetary boundary layer and lower troposphere.

#### **#502 - Measurements of differently-sized volcanic particles for understanding eruptive processes: the 12-13 January 2011 lava fountain case from Mt Etna, Italy**

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Mt Etna, in Italy, is one of the most active volcanoes in the world. In the last 20 years, more than 200 paroxysmal episodes occurred from one of its summit craters, with a style of activity which spans from Strombolian to lava fountaining. The 12-13 January lava fountain took place from the New South-East Crater, and produced tephra fallout extended to more than 100 km SSW from the vent. Sampling carried out along the axis of the entire deposit has allowed to collect volcanic particles ranging in size from bombs to fine ash, i.e. between more than 20 cm and less than 0.1 mm. On these particles, as a function of their size, we carried out different types of measurements, including clast density, morphological and textural investigations, and chemical analysis. By using the method of the three orthogonal maximum dimensions ( $A > B > C$ ), over the proximal deposit we measured: a) >140 largest clasts (in the range 16-2 cm) from 14 sites to evaluate the eruption plume dynamic close to the vent, and b) 1500 clasts (8-32 mm) from 9 representative sites, in order to investigate the 3D shape of the lapilli class. Density measurements of 200 lapilli-sized particles were carried out by hydrostatic weighing on an electronic balance allowing to describe the vesicularity of the magma. The ash-sized class (particles <2 mm) was selected for componentry and morphological analyses, both under binocular stereomicroscope and scanning electron microscope (SEM). Results can be discussed in terms of what types of volcanic particles were produced during the eruption and how their textural features vary with respect to the distance of sampling from the vent. Mineralogical and textural observations of thin sections have been made under petrographic microscope, aimed at deriving information on the percentage of the different microlite phases. Finally, glass compositions on the ash particles (performed by SEM analysis) indicated variations in magma composition. The combination of different results obtained through the whole set of measurements and analyses represent the only tool to give insights into the main eruptive processes which accompanied the 12-13 January lava fountain. We will discuss them in terms of magma ascent and fragmentation in the conduits, terminal settling velocity and fallout in the ground.

#### **#503 - DRAG COEFFICIENT OF NON-SPHERICAL PARTICLES**

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We present a new model for the prediction of the drag coefficient of non-spherical solid particles that is valid in the range of particle Reynolds numbers  $Re < 10^5$  (i.e. creeping to turbulent regimes). Results are obtained from analytical solutions for particles moving at  $Re \ll 1$  and experiments on 300 regular and irregular particles both in settling columns with heights between 0.45-3.6 m ( $10 < Re < 300$ ) and a 4-meter high vertical wind tunnel ( $10^4 < Re < 10^5$ ). Size and shape of particles are characterized by using 3D laser scanning, SEM micro-CT and image analysis. Our analyses show how none of existing shape descriptors, such as sphericity, circularity, elongation and flatness, well correlate with the particle drag coefficient. We introduce two new and easy-to-measure shape descriptors, namely Stokes' and Newton's shape descriptors, which are functions of particle form only (i.e. flatness and elongation) and have the highest correlation with the drag coefficient. Our results also indicate that orientation of non-spherical particles can significantly affect the drag coefficient. In particular, at high Reynolds numbers ( $Re > 1000$ ), the particle to fluid density is the key parameter controlling the particle orientation and, hence, the drag coefficient. As a result, effect of density ratio and particle orientation are added to our new model. In addition, effects of surface roughness (or surface vesicularity) on the drag coefficient of non-spherical particles at various Reynolds numbers are investigated and its effect on the drag coefficient is found to be negligible. We have also found that existing spherical and non-spherical models are associated with an average error of 30% for estimating settling velocity of volcanic particles, while for highly non-spherical particles their errors can be significantly higher. Benchmark tests show that our new model is reliable and easy to apply for estimating drag coefficient of non-spherical particles of various shapes in a wide range of particle to fluid density ratio and Reynolds numbers.

#### **#504 - Advanced GPS products for Volcanoes Monitoring applied at Mount Etna**

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The GPS electromagnetic waves that propagate in the neutral atmosphere are perturbed by the local characteristics of the crossed medium. Variations of pressure, temperature and water content, together with the presence of hydrometeors and particulates, cause changes in the refractive index along the ray path. Since 1988, the Istituto Nazionale di Geofisica e Vulcanologia (INGV-OE) monitors ground deformation at Mt. Etna. Nowadays, the network geometry consists of 42 permanent stations that provide a dense coverage of the volcano edifice. Owing to both the high frequency of explosive episodes and the well-developed GPS network, Mt. Etna is particularly suited for an in-depth investigation into the potential of GPS technique in the volcanos monitoring. Two main issues have been addressed: the wet tropospheric tomography to improve the precision of the Differential Interferometry Synthetic Aperture Radar (DInSAR) technique and the capability of GPS in detecting the volcanic plumes. The DInSAR technique, used in geodesy to monitor the volcanic areas, is affected by atmospheric artefacts that are the most significant and, probably, the most difficult to identify and reduce. Due to the prominent topography of Etna volcano and the quite variable weather conditions, the atmospheric heterogeneities become even more pronounced. The estimation of atmospheric anomalies using GPS measurements have noticeable importance to establish the "effective" ground deformation of the volcanic edifice. A software has been developed for deriving the tropospheric tomography starting from the GAMIT software output. The wet refractivity tomography was applied on experimental data of DInSAR Sentinel1 IW on Mount Etna. Concerning the second topic, in the last years the Mt. Etna high frequency explosive activity formed volcanic plumes that rose up to kilometres above the vent. We investigate the ability of GPS to detect volcanic plumes at Etna through the analysis of the GPS Signal to Noise Ratio (SNR) data. The SNR data provide no information about the distance between the satellite transmitting the signal and receiver, and thus make no direct contribution to positioning solutions. However, the SNR data are important because they can directly measure signal attenuation or blockages. We develop and test the method on the volcanic plume produced during some explosive episodes. Results show that, during the eruption, the SNR data had a drop caused by the presence of dense ash-laden plumes.



**#505 - Gel dosimeters for medical physics applications**

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Gel dosimeters for three-dimensional mapping of radiotherapy doses were introduced at Yale University in the mid-1980's. Soon after, R&D in this field also started in Italy. Early work was done at the Istituto Superiore di Sanità, and at the Universities of Pisa and Milan. Several institutes now collaborate on this topic with support from the Italian Ministry for University and Research (MIUR) through Grant PRIN SNALEM2010 "Development and application of new materials for ionizing radiation dosimetry". This presentation describes this research, which aims at developing new formulations of hydrogel matrices with improved characteristics of stability, sensitivity and spatial resolution compared to those of earlier Fricke-gel and polymer-gel systems. An additional goal of our research is the simplification of the manufacturing processes in order to facilitate the diffusion of this technology and its transition from the bench to the bedside.

**#506 - Hadrontherapy: from the conventional modality to the laser-driven approach**

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External radiation treatments coupled to (on-line and off-line) imaging techniques with hadron beams represent, nowadays, the frontier of conformational radiotherapy for tumor treatments and one of the best clinical approach for the battle against cancer. Today, more than 40 hadrontherapy centers are active around the world and about 40 are planned to be realized in the next five years.

Nevertheless, the large-scale adoption of hadrontherapy centers is strongly limited by the complexity and cost of these facilities. In this context, laser-accelerated ion beams represent a fascinating alternative in the field of non-conventional acceleration techniques. The INFN ELIMED (ELI-Beamlines MEDical and multidisciplinary applications) project aims to demonstrate the potential medical applicability of optically accelerated proton beams.

In this work we will present the status of the art of the clinical dosimetry with proton beams as well as the future challenges that the laser-driven beams reserve in this field.

Design, development and characterization of beam transport, selection and dosimetric devices for high-energy laser-driven proton beams will be also presented.

**#507 - Innovative approaches in the dosimetry of laser-driven proton beams for future hadrontherapy applications**

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Over the last decades, charged particle acceleration using ultra-intense and ultra-short laser pulses has been one of the most attractive topics in the relativistic laser-plasma interaction research. Actually, one of the most challenging ideas consists on using laser-target interaction as a source of high-energy ions for medical applications. In this framework, the purpose of the international ELIMED network consists on demonstrating that laser-driven high-energy proton beams can be used for multidisciplinary applications investigating, particularly, new approaches in the hadron-therapy field.

We started to design a beam transport line prototype that allow the focalization and selection of the accelerated particles able to deliver laser-generated proton beams with optimized properties suitable for multidisciplinary applications.

Furthermore, a Faraday cup (FC) prototype for absolute dosimetry has been designed and realized and preliminary tests have been performed with conventional proton beams at LNS-INFN, and with laser-driven beams at the PALS laser facility in Prague and at the TARANIS laser facility in Belfast.

In this contribution, the design and development of the dosimetric prototypes developed will be discussed. Moreover, preliminary results obtained at the mentioned facilities will be presented.

**#508 - A GEANT4 Monte Carlo application to simulate a laser-driven electron beam line**

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The laser-driven accelerator (LDA) based on the Laser Wake-Field Acceleration [1] mechanism in plasmas are now entering in a mature phase (see L. Labate abstract), so that they can be considered, in perspective, as alternatives to the RF LINACs for the medical practice, and in particular for radiotherapy [2].

Over the past few years, laser-driven electron accelerators have evolved greatly; they are able to produce electron bunches with energies up to tens MeV, thus representing a new option for medical application as the Intra-Operative Electron Radiation Therapy (IOERT). The use of a LDA for IOERT would allow a much smaller device to be introduced into the operating room, as the most bulky component, the laser system, may be placed and monitored outside.

Important different characteristics of a LDA respect to a conventional clinical accelerator, require accurate studies related to dosimetric and biological issues. To conduct biological and preclinical research activities and to study the radiobiological effectiveness of these very intense pulses, it is necessary to obtain a dosimetric characterization of the electron beam.

This characterization can be validated with a Monte Carlo simulation tool, based on the GEANT4 toolkit, developed especially for a LDA.

GEANT4 is a toolkit for the simulation of the passage of particles through matter [3]. It allows the particle tracking during their motion, create geometrically the physical system and recreate the physical processes. It also includes a large set of materials and elements to allow the reconstruction of the system as close as possible to the real one.

We have analyzed the dosimetric characterization of the electron beam by comparing numerical simulations with real measurements carried out utilizing the LDA installed at National Institute of Optics (INO) of CNR Pisa [4].

From the GEANT4 simulation analysis, the energy distribution and angular spread of the beam were evaluated. Moreover, 2D distribution and 3D profile of the dose and PDD curves were obtained. The GEANT4 application could be used to provide the appropriate data about the experimental set-up to carry out biological experiments [4].

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[4] D. Lamia et al., *Nuclear Instruments and Methods in Physics Research A* 786 (2015) 113–119

**#509 - EXPERIMENTAL NANODOSIMETRY: THE LINK TO RADIOBIOLOGY**

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The biological effectiveness of ionizing particles is clearly related to their track-structure properties on a nanometric scale. It was therefore the aim of this work to develop a method and a detector which allow to measure directly the track structure properties of light ions of therapeutic interest.

The track-nanodosimeter installed at the TANDEM-ALPI accelerator complex of LNL (Legnaro National Laboratories) counts the number of ionizations produced inside a small gas volume by ionizing particles directly crossing it, or passing nearby at given impact parameter. From the point of view of ionizing interactions, the gas volume simulates a cylindrical water target volume of nanometric dimensions. For a detailed description of the experiment see ref. [1].

Considering the great interest for light ions in radiotherapy, the study of particle track structure properties was concentrated on protons, Li-ions and C-ions. Ionization cluster-size distributions were measured and simulated by a dedicated Monte Carlo simulation code. Some descriptors of the track structure can be derived from these distributions. They describe particular aspects of the track structure of ionizing particles and hence also of radiation quality.

In analysing the large amount of data collected during the last years, the main attention was focused on particular properties of the ionization cluster size distributions, the first moment  $M_1$ , representing the mean number of ionizations produced in the target volume  $V$  at the passage of the ionizing particle at given impact parameter, and the corresponding cumulative probability  $F_k$  of measuring cluster sizes  $n \geq k$ .

It was found that the sum distributions  $F_k$  behave, as a function of  $M_1$ , similarly to the radiobiological cross sections as a function of *Linear Energy Transfer* (LET), first increasing with increasing values of  $M_1$  and then showing a saturation effect.

When also radiobiological data are plotted as a function of the mean ionization-cluster size  $M_1$ , the result is a clear relation between radiobiological cross sections and some of the cumulative distributions  $F_k$ . The correspondence between radiobiological cross sections and experimental nanodosimetric data for protons and carbon ions will be presented.

#### #510 - The impact of self-oxidation on the dosimetric performance of ferrous-sulfate/xyleneol-orange gels

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Since their introduction in the 1980's, most of the research on ferrous-sulfate gel dosimeters has aimed at minimizing the ferric ion diffusion phenomena that blur the 3D distribution of the signal. However, equally important are the spontaneous oxidation effects, which alter the sensitivity of the gels over time. In some gels, this effect is very pronounced and must be accounted for even when production, calibration and use of the gels are separated by just a few days. In other cases, the effect is much milder, but should still be properly accounted for when gels are used over a long period a time, such as in the proposed monitoring of adaptive radiotherapy treatments. Our work examined and modeled the spontaneous oxidation processes occurring in ferrous-sulfate/xyleneol-orange gels for 3D dosimetry. The model accounts for the time interval between production of the gels and their use, as well as for the fractionation schemes adopted for the irradiations. Based on a single kinetic constant and on the initial amounts of Fe<sup>2+</sup> and Fe<sup>3+</sup>, our model predicts as a function of time the amount of Fe<sup>3+</sup> present in the gels and coordinated with xyleneol-orange.

#### #511 - Use of alanine EPR dosimeters for discriminating neutron and photon components in the thermal column of Pavia Triga reactor

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The optimization of the procedures of Neutron Capture Therapy (NCT) for cancer treatments involves research for beam characterization. One major issue for this therapy is the reliable dosimetric determination of the various (neutronic and photonic) components of the employed beam. In particular, the precise and accurate measurements of the gamma photon component is fundamental for evaluating the risks to healthy tissues hit by the mixed field.

Among solid state dosimeters the alanine detectors read by Electron Paramagnetic Resonance (EPR) technique present several advantages such as: tissue equivalence for photon and electron beams, linearity of its dose-response over a wide range, high stability of radiation induced free radicals, no destructive read-out procedure, no sample treatment before EPR signal measurement and low cost of the dosimeters.

These features associated with the possibility of recognizing the various components of a mixed radiation fields makes alanine a good candidate for dosimetry in neutron-gamma fields.

In this work we determine the gamma component of the mixed radiation field in thermal column of the Triga Reactor of University of Pavia (which is used for experimental activities on NCT) by means of alanine EPR dosimeters.

Commercial alanine dosimeters produced by Synergy Health (Germany) were exposed in three positions in the thermal column; the irradiations were performed inside graphite holders to avoid use of hydrogenous phantoms for minimizing the gamma contribution due to the plastic holders. EPR measurements were carried out through Bruker ECS106 spectrometer equipped with a TE<sub>102</sub> rectangular cavity. In order to isolate the gamma components of the mixed field two kinds of irradiations were carried out inside a lithium carbonate box (wherein the thermal neutron component is heavily reduced) and outside of it.

MCNP Monte Carlo simulations of the irradiation set-up were carried out, calculating the contributions of the various components present in the mixed field (thermal and fast neutron and gamma).

The experimental values are compared with the computations of the Monte Carlo simulations and the results are discussed on the basis of the mixed field features and on the response of alanine dosimeters to high and low LET radiations.

#### #512 - Alanine EPR pellets for dosimetry of clinical proton and carbon ion beams

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Proton and carbon ion beams offer several advantages compared to other radiation fields for therapy such as low lateral scattering and high biological effectiveness (RBE) in the Bragg peak region, making them particularly attractive for the treatment of radio-resistant tumors localized close to organs at risk. Although ion beam radiotherapy ultimately requires dose prescription in terms of biological dose or cell survival, absorbed dose is still the quantity mostly used in clinical quality assurance and to dosimetrically characterize the beam.

Among solid state detectors the alanine EPR detectors present several advantages such as: tissue equivalence, linearity of its dose-response over a wide range, high stability of radiation induced free radicals, no destructive read-out procedure, no sample treatment before EPR signal measurement. These features associated with the possibility of recognizing the various components of a mixed radiation fields makes alanine a good candidate for Quality Assurance of clinical particle beams.

The main goal of the present work is to investigate the response behaviour of alanine EPR pellets in clinical proton and carbon ion beams. Proton irradiations were carried out at PSI (Switzerland) using both passive and active scattering modality, whereas,  $^{12}\text{C}$  ions irradiation were performed at GSI (Germany) adopting the raster scanning modality.

Regarding the passive scattering modality, Output Factor measurements have been carried out at the OPTIS2 facility of PSI and the results are in agreement with Hi-p semiconductor diode up to 10 mm collimator diameter. Moreover, regarding the active scanning technique (raster scanning for  $^{12}\text{C}$  and spot-scanning for protons) the alanine response at selected locations in depth has been measured and compared with TPS planned dose in different quasi-clinical scenarios. A dosimeter 'quenching' more evident for  $^{12}\text{C}$  ions than for protons was measured.

Furthermore, the study of EPR signal stability after irradiation was performed for both proton and carbon ion irradiations.

#### **#513 - Fricke gel layer dosimeters for measurements of all dose components in irradiations with epithermal neutrons beams at a research reactor**

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Gel dosimeters in form of layer have shown noticeable potential for dosimetry in epithermal or thermal neutron fields with very high fluence rate, as those characteristic of nuclear research reactors that are exploited for boron neutron capture therapy (BNCT), because they give the possibility of attaining the spatial distribution of the various dose components generated by neutron reactions in water-equivalent phantoms.

Wide studies have been carried out utilising laboratory-made Fricke gel dosimeters containing xylenol orange. By suitably adjusting the dosimeter isotopic content, the separation of the dose components having different LET can be achieved. In their standard composition, these dosimeters are water equivalent for neutrons and for all the secondary radiations generated by neutron reactions inside the phantom. In particular, the dose due to the charged particles generated by the reactions of thermal neutrons with  $^{10}\text{B}$  can be attained from the dose images obtained with two dosimeters, a standard one and another containing a suitable amount of  $^{10}\text{B}$ . From the boron dose images, the thermal neutron fluence images can be attained by means of the kerma factor. The gamma dose and the dose due to fast neutrons, not negligible in the case of epithermal neutron beams, can be separated by suitable elaboration of the dose images measured by means of two other dosimeters, a standard one and another with the same chemical composition but prepared with heavy water.

Fricke-xylenol-orange gel dosimeters have also shown to be a valid aid for the characterization of the neutron beams from epithermal or the thermal columns of a research reactor.

**#514 - Manipulation of hyperentangled and cluster states via integrated photonics**

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Encoding many qubits in different degrees of freedom (DOFs) of single photons is one of the routes towards enlarging the Hilbert space spanned by a photonic quantum state. Hyperentangled photon states (i.e. states showing entanglement in multiple DOFs) have demonstrated significant implications for both fundamental physics tests and quantum communication and computation. Increasing the number of qubits of photonic experiments requires miniaturization and integration of the basic elements and functions to guarantee the set-up stability. This motivates the development of technologies allowing the precise control of different photonic DOFs on a chip. We demonstrate the simultaneous control of both path and polarization DOFs of a photon pair in an integrated quantum circuit fabricated by femtosecond laser writing. We tested the properties of four-qubit linear cluster states built on both DOFs. Our results pave the way towards the full integration on a chip of hybrid multiqubit multiphoton states

**#515 - Non-adiabaticity and entropy production in quantum thermodynamics processes**

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We study the out-of-equilibrium thermodynamic properties of unitarily evolving quantum systems (driven by a time dependent control parameter entering their Hamiltonian) and in particular compare the work actually done on the system with the adiabatic one, that would be performed following an infinitely slow protocol. The non-adiabatic part of the work, called *inner friction*, can be used to reveal irreversibility in the process and is intimately linked to the non-equilibrium entropy production. Indeed, it can be expressed as the relative entropy between the actual state of the system and the ideal one, and it is associated to a specific fluctuation relation for the entropy production, which allows the inner friction to be expressed in terms of its cumulants. We apply this formalism to various cases of experimental relevance, showing explicitly that the inner friction is linked to the speed at which the process is performed and to the diabatic transitions that occur in the system.

Reference

F. Plastina et al. , Phys. Rev. Lett. 113, 260601 (2014).

**#516 - Quantum control of two-qubit gates via dynamical decoupling filtering of 1/f noise**

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Achieving high-fidelity universal two-qubit gates is a central requisite of any implementation of quantum information processing. In solid-state nanocircuits, noise with 1/f power spectrum represents a severe obstacle towards this goal [1]. For single-qubit gates considerable improvement has been achieved by operating at optimal points and further enhancement has been obtained by open-loop dynamical decoupling. However, protection of qubit coherence during a multi-qubit gate poses non-trivial additional problems. In fact decoupling may disrupt the inter-qubit dynamics thus conflicting with gate operation. Here we present the integration of dynamical decoupling into a universal two-qubit gate in the presence of 1/f noise acting locally on each of the qubits forming the entangling gate. We address both the case of pure dephasing and of depolarizing noise and investigate the gate efficiency under periodic, Carr-Purcell, and Uhrig dynamical decoupling sequences.

Our analysis is based on the exact numerical evaluation of gate operation for 1/f noise measured in superconducting qubits and on perturbative (Magnus) expansion for quasi-static noise. For transverse noise we find that a threshold value of the number of pulses exists above which the gate error is reduced as  $n^\alpha$  with  $\alpha$  depending on the dynamical decoupling sequence. For smaller pulse numbers, dynamical decoupling may even increase the error with respect to the unconditioned evolution, a behavior reminiscent of the anti-Zeno effect. For pure dephasing noise we find an analytic expression of entanglement fidelity in terms of noise filter functions allowing to single out the sequence-specific capability to bypass cumulants of the underlying non Gaussian processes. The possibility to reach the accuracy threshold for fault-tolerant quantum information processing with solid-state devices by quantum gates with integrated decoupling is critically discussed.

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**#517 - Thermal current and dephasing in a fluxonium qubit**

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Thermal currents through Josephson junctions are carried by quasiparticles above the gap and depend on the superconducting phase difference across the junction through Andreev reflection processes. This has been experimentally verified a few years ago, where the thermal current due to a temperature gradient across a two-junction SQUID has been measured. While this is of relevance for the coherent tunability of thermal currents on one hand, we have shown that it also has an impact on devices containing Josephson junctions, where accidental temperature gradients can occur. We have investigated the impact of very small thermal gradients on a fluxonium qubit, and to do that we have used the thermal current in the linear response regime. This fluxonium, which is a superconducting qubit consisting of a SQUID with multiple Josephson junctions, has the unique advantage of being protected against both charge and flux noise. In particular is well protected against flux noise thanks to its array of Josephson junctions which acts as a superinductance. We have shown that the thermal currents have a measurement character on the state of the qubit. In other words, the thermal currents contribute to limiting the dephasing time of the qubit, according to the temperature of the system. We have shown that the sensitivity of the thermal current to the qubit states is independent on the number of junctions in the array of the superinductance. Moreover, we have shown that the superinductance, which results in a small inductive energy, gives a good protection also to thermal dephasing.

### #518 - Functional approach to heat-exchange, application to the spin boson model: from Markov to quantum noise regime.

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The emerging field of quantum thermodynamics aims to extend basic concepts of thermodynamics at the nanoscale. Indeed lowering the dimension of a system, fluctuations and quantum effects become crucial and classical thermodynamics cannot be simply applied. The question of how a small system exchanges heat and energy with a bigger one is very important both from technological and fundamental point of view. A deep understanding of heat exchange at the nanoscale is necessary in view of the realization of quantum devices such as quantum heat engines which could have great technological impact. Despite much recent efforts, the thermodynamics of quantum systems is still poorly understood, at least when compared to its classical counterpart. Here we aim to go a step forward towards a microscopic and rigorous description of heat exchange in quantum system.

We face with a path-integral approach the problem of a quantum system coupled to a thermal reservoir and consider the energy flows between them.

In this framework we can write a general heat influence functional which embodies all the dissipative mechanisms and allows us to study heat processes.

We present the exact formal solution for the

moment generating functional which carries all statistical features of the heat exchange process for general linear dissipation.

As an application we study the paradigmatic case of a two-level system and we show that at low temperature non-Markovian effects could dominate the time evolution of the average heat and heat power.

### #519 - Out-of-equilibrium Thermodynamics of Quantum Optomechanical Systems

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The exploration of out-of-equilibrium features of small systems is attracting an ever-increasing attention.

Given the spectacular level of control achievable over smaller and smaller systems, one would eventually reach a point where quantum fluctuations — besides thermal ones — start playing a non-negligible role. In particular, optomechanical systems seem particularly suited to enquire that regime, and offer the unique perspective of bridging the study of quantum thermodynamics with the macroscopic domain. However this requires an adequate analysis — pursued at a fully quantum level — of the thermodynamical properties of the optomechanical interaction, in particular retaining the nonlinearity of the interaction at the level single-photon coupling. With these motivations we explore and characterize the thermodynamical behavior of an optomechanical system driven out of equilibrium by a time-dependent transformation. We address an isolated quantum system, consisting of an optical mode confined in a cavity and parametrically coupled to a mechanical oscillator, evolving according to a time-dependent Hamiltonian and undergoing a two-step measurement protocol. We access analytically the full distribution of the

work generated by the process, addressing both linear and quadratic optomechanical coupling, where the cavity field is parametrically coupled to either the position or the square of the position of a mechanical oscillator, respectively. In the former case we find that the average work generated by the quench is zero, whilst the latter leads to a non-zero average value. Through fluctuations theorems we access the most relevant thermodynamical figures of merit, such as the free energy difference and the amount of irreversible work generated. We thus provide a full characterization of the out-of-equilibrium thermodynamics in the quantum regime for nonlinearly coupled bosonic modes. Our study is the first due step towards the construction and full quantum analysis of an optomechanical machine working fully out of equilibrium.

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**#520 - Using The Virtual Brain simulation framework as a Technology and Development platform for medical applications**

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The Virtual Brain is a whole brain simulation platform (thevirtualbrian.org). It provides a unifying mathematical framework for multimodal brain data including functional and structural neuroimaging data. An automated processing pipeline allows preprocessing imaging data of different modalities, precisely aligning them and using them as model constraints. This way each model can be personalized by integrating individual patient data. We are currently testing The Virtual Brain for epilepsy and stroke patients and using it in combination with mobile EEG technology to improve decoding brain states in real life scenarios. The Virtual Brain can be used as a mathematical microscope to reveal internal states and processes that cannot be captured by noninvasive imaging methods alone. For example it is capable to generate new hypotheses on complex mechanisms underlying plasticity and learning taking into account complex network interactions that otherwise would be difficult to keep track on. In addition the standardized modeling framework guarantees reproducibility of simulations and testing as well as comparison of a wide range of different model classes which allows identification of generic models that capture a maximum range of dynamical regimes of the brain under a multitude of different conditions.

**#521 - Boron-doped nanocrystalline diamond microelectrodes for detecting amperometric and potentiometric signals from excitable cells**

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Thin-films of synthetic boron-doped diamond (BDD) grown on insulating substrates allow the fabrication of electrochemical biochips with unmatched performances thanks to the extreme properties uniquely possessed by diamond mechanical. The most common substrate for BDD-devices is silicon, due to its chemical and thermomechanical compatibility with diamond. Unfortunately, this material is opaque in both the visible and UV-range. Aiming at simultaneous electrochemical and fluorescence detections of biological events, we developed a new diamond-on-glass technology, which yields diamond films of good conductivity and at the same time allows to reach a transparency of ~ 50 % in the visible and near-UV range. Based on this technology, a variety of Microelectrode Arrays (MEA), with layouts ranging between 4 and 64 independent microelectrodes has been successfully fabricated.

Being Diamond an excellent material for RedOx (type-0) electrodes, those chips are primarily committed to the amperometric detection of catecholamine release from chromaffin cells. In this application, they show excellent sensitivity, very low noise, fast response and long-life. Moreover, by characterizing electrochemically the diamond MEAs, it turned out that our devices are also suitable for potentiometric detection, provided tailored read-out electronics is available. This approach conducted to successful recordings of action and field potentials and even transient pH-variations.

Our last developments are focusing on enhancing the detection sensitivity, aiming at applications with dopaminergic neurons. For this purpose, the BDD-electrodes require a lower impedance and at an enhanced electrochemical activity. In order to achieve these goals, we investigated two approaches to provide a 3D nanostructuring of the electrodes surface. One is based nanowires, the other on a porous conducting polymer. Furthermore, the instrumentation setup includes now, beside the traditional chronoamperometry operation, also the fast-scan cyclic voltammetry (FCV), which allows the simultaneous detection of different redox species with a time-resolution of ~100 ms.

**#522 - Diamond based-electrochemical sensor for simultaneous detection of quantal exocytic events from neuroendocrine cells**

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The study of the mechanism involved in the observed catecholamine (i.e. adrenaline) secretion is of paramount importance in neuroscience research in order to achieve a better understanding of the signal transmission among neurons. New technologies allow overcoming the limitations of current standard approaches. Diamond-based sensors, taking advantage of the extreme properties of this material (biocompatibility, chemical inertness, single defects quantum properties), represent the next generation devices.

In the present work we report about a systematic investigation of quantal exocytic events from cultured bovine chromaffin cells carried out by a diamond-based Multi Electrode Array (MEA) sensor.

The biosensor was fabricated using an opportunely masked broad 1.3 MeV He<sup>+</sup> ion beam on a IIa monocrystalline diamond sample (4.5×4.5×0.5 mm<sup>3</sup>). This process provides buried highly conductive graphitic channels (resistivity ~mΩ·cm) embedded in a highly insulating and chemically inert diamond matrix which can act as electrochemical sensors for excitable cells, as already demonstrated by amperometric measurement of exocytic events on single-electrode device [Adv.Mat2013] and by a preliminary characterization of the multi electrode sensors.



Taking advantage of the biocompatibility of diamond, cultures of chromaffin cells were incubated over the surface of the device. Quantal secretory responses were simultaneously measured from stimulated cells positioned on the 16 graphitic microelectrodes. The proposed diamond based sensor exhibits sensitivities toward oxidizable molecules similar to that of standard commercial techniques, as demonstrated by the full compatibility of the presented results with those obtained using carbon fibre microelectrodes. However, our new device offers a faster data harvesting due to the multi electrode integration and the possibility of recordings from cell populations, thus using the microchip for fast drug screening over a large number of biological samples.

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[Sensors-Basel2015] F. Picollo et al. *Sensors*, 15 (2015) 515

### #523 - Towards innovative bioimaging techniques exploiting NV centers in nanodiamonds

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Nitrogen Vacancy (NV) centers in nano-diamonds (ND) have many interesting characteristics that renders them promising tools for nano and quantum technology applications, these range from the realization of on demand deterministic single photon sources to the implementation of quantum information protocols.

In recent years, among the other appealing properties of NV-ND, their bio compatibility has emerged with increasing evidence as well as their functionality under physiological conditions, so that they can effectively safely pass the cell membrane for intracellular biosensing purposes.

In this talk we discuss the preliminary results obtained in the exploitation of magneto-optical detection of spins associated to NV centers in diamond for new bioimaging techniques at room temperature at the nanometric scale.

### #524 - Memristive behavior in nanoscale metal oxides

Carlo Ricciardi - *Politecnico di Torino*

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The discovery of memory-resistors (memristors) represents one the latest breakthrough in fundamental electronics and physics. Memristors are two-terminal passive electronic devices, with a resistance that dynamically changes depending on the previous usage, and that can be maintained over time, similarly to what happens in brain's synapses. The interest in the memristor area is therefore rapidly increasing for the high potential to emulate the behavior of real neural circuits in high-power computing and neuromorphic learning systems.

Metal oxides such as titanium and tantalum oxide have shown resistive switching behavior when applied as nanometrically thin layers inside metal/insulator/metal structures. Furthermore, nanostructured metal oxides such as ZnO nanowire-based systems are predicted to achieve significant breakthroughs in memristive devices, because they present large interfacial area and direct charge conduction path, which are important features for resistive switching applications.

TiO<sub>x</sub> and TaO<sub>x</sub> thin films were deposited by atomic layer deposition (ALD) at different temperatures, while ZnO nanowire/polymer core-shell structures were achieved thanks to Chemical Vapour Deposition (CVD) and Plasma Polymerization techniques. Electrical, structural, morphological and compositional properties of such materials will be discussed in view of elucidating their memristive behavior.

### #525 - Parco Area delle Scienze 37/A - 43124 Parma, Italy

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Organic and Organic Bio-hybrid Memristive Devices

Organic based biosensing and memristive devices are more and more paving the way to novel perspectives both in mimicking and interfacing natural systems while representing an ideally suitable platform for applications in bio-electronics and bio-medicine. Our contribution to the field including applications to drug delivery studies and bioelectronics will be introduced and discussed together with the recent achievements in developing memristive devices based both on PANI/PEO and PEDOT::PSS polymers. The evolution

from simple logic elements up to the first organic based Perceptron will be discussed envisaging the perspective. The results and potential of the approach based on organic electrochemical devices, as well as a comparison with methods already established in the field, will be discussed together with the great potential of these devices. The novel approach based on interfacing memristive devices with biological cells and systems will be introduced together with the demonstration of a memristive organic-bio-hybrids that will be proposed and discussed as a potential for novel very promising applications.

VA Demin, VV Erokhin, AV Emelyanov, S Battistoni, G Baldi, S Iannotta, Hardware elementary perceptron based on polyaniline memristive devices *Organic Electronics* (2015 in press).

A.Romeo, G.Tarabella, P.D'Angelo, C.Caffarra, D.Cretella, R.Alfieri, P.G.Petronini, S. Iannotta Drug-induced cellular death dynamics monitored by a highly sensitive organic electrochemical system. *Biosensors and Bioelectronics* 68, 791-797 (2015)

G. Tarabella, P. D'Angelo, A. Cifarelli, A. Dimonte, A. Romeo, T. Berzina, V. Erokhin and S. Iannotta A hybrid living/organic electrochemical transistor based on the *Physarum polycephalum* cell endowed with both sensing and memristive properties *Chem. Sci.* 6, 2859-2868 (2015)

#### #526 - Synchronization phenomena in oscillatory neural networks with memristor synapses

*Fernando Corinto - Politecnico di Torino*

The memristor manifests qualities and behaviors which are naturally observed in biological synapses. It exists at the nano-scale, it consumes very little power, it is ideally suited for parallel processing, it may process and store information simultaneously, and, last but not least, it offers a conductive behavior depending on the time evolution of the flux through it.

Furthermore it is able to reproduce rules governing the process of neural learning, including the Hebbian rule, Spike-Time-Dependent-Plasticity and Spike-Rate-Dependent-Plasticity.

Recent studies confirm that the nanoscale memristor is a serious candidate to become the core element of novel neuromorphic systems due to its ability to emulate the behavior of a biological synapse more efficiently and accurately than any conventional electronic circuit.

This manuscript aims to provide some insight into the mechanisms underlying the emergence of synchronization in oscillatory neural cells (e.g. Hindmarsh-Rose neurons) coupled through memristors. Extensive numerical investigations show that in some cases the nonlinear dynamics of the memristor play a key role in the development of synchronous oscillations in the network. The results are then confirmed by theoretical analysis based on the contraction mapping theory.

This work sheds light on some aspects of the nonlinear behavior of the still largely unexplored memristor, which is doomed to make an impact in integrated circuit design in the years to come.

#### #527 - Pulsed laser deposition of ZnO and VO<sub>2</sub> films for memristor fabrication

*Giuseppe Lullo - Dipartimento di Energia, Ingegneria dell'Informazione e Modelli Matematici (DEIM), Università di Palermo*

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Memristors are resistive switching memory devices which have attracted much attention over the last years for high-density memory applications because of their simple structure, small cell size, high speed, low power consumption, potential for 3-D stacking and excellent compatibility with the complementary metal-oxide-semiconductor (CMOS) technology [1]. Beside nonvolatile memory applications, memristors have been also proposed for other different applications including biosensors [2] and neuromorphic [3] circuits.

The device structure is simply an oxide material sandwiched between two metal electrodes. The switching behavior is not only dependent on the oxide material but also on the choice of metal electrodes and their interfacial properties. For this reason switching characteristics of many metal oxide films (e.g. TiO<sub>2</sub>, NiO, TaO<sub>2</sub>, HfO<sub>2</sub>) and metal contacts have been studied [1]. ZnO has attracted much attention as oxide material for resistive switching application, due to its abundance in nature, which means low cost, and compatibility to CMOS technology [4] in terms of process integration and device scalability down to nanometric sizes. VO<sub>2</sub> is also a promising candidate as switching element for data storage [5].

In this work we report on the fabrication and electrical characterization of microscale ZnO and VO<sub>2</sub> memristors. ZnO-based memristors have active areas ranging between 2 × 2 mm<sup>2</sup> and 300 × 300 mm<sup>2</sup>. VO<sub>2</sub>-based memristors have instead dimensions between 100 × 100 mm<sup>2</sup> and 300 × 300 mm<sup>2</sup>. Both oxides were deposited by pulsed laser deposition (PLD) on FTO (Fluorine-Tin-Oxide) glass substrates at the conditions reported in [6]. After the oxide deposition, top metal contact were defined by direct laser-writing microlithography and subsequent lift-off. All devices were electrically characterised at room temperature by performing two-probe I-V measurements by means of a custom developed electronic circuit. For all devices the typical I-V curve of hysteresis was achieved by sweeping the applied voltage in the range -3 to 3 V.

An analysis of the high resistance state (HRS) and low resistance state (LRS) against the device size showed that for both material systems the LRS is independent on the device area, suggesting that the ON-state of the device is dominated by a local, filamentary

phenomenon. Moreover, smaller devices exhibit a HRS increasing with device size decreasing. Finally, ZnO devices have proven to be more suitable for memory application than VO<sub>2</sub>-based device, exhibiting a higher R<sub>OFF</sub>/R<sub>ON</sub> ratio.

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**#528 - the redefinition of the international system of unit***Giovanni Mana (I) - INRIM**Other Authors: E. Massa - INRIM*

Metrologists are considering to redefine the international system of units by assigning conventional values to a set of fundamental constants; this will be the greatest change after the introduction of the metric system. All the units are under scrutiny, but the kilogram is in the spotlight. This contribution illustrates the metrologists' effort to align the international system with our present view of reality, with particular emphasis on the kilogram redefinition. It reviews the measurements of the Avogadro and Planck constants describing how the experiments which deliver the most accurate values of these constants are realizing the kilogram by counting silicon atoms to within the  $2 \times 10^{-8}$  relative accuracy necessary to ensure the continuity of mass metrology.

**#529 - Precision measurement of the Newtonian gravitational constant by atom interferometry***Gabriele Rosi (I) - INFN, LENS and Florence University**Other Authors: Guglielmo Maria Tino, Fiodor Sorrentino, Giulio D'Amico (Dipartimento di Fisica e Astronomia & LENS Università di Firenze, INFN Sezione di Firenze), Luigi Cacciapuoti (European Space Agency Research and Scientific Support Department), Marco Prevedelli (Dipartimento di Fisica dell'Università di Bologna)*

The accurate determination of the Gravitational Constant  $G$  has always been a challenging task. After 300 different measurements, starting from the original one performed by Cavendish in 1798, the  $G$  value still now presents a large relative uncertainty compared to all other physical constants. In order to detect systematic effects that plague such measurements the use of different methods with respect to the traditional ones is crucial. Here we report on the first precise determination of  $G$  using microscopic test masses in free fall (cold Rubidium atoms) and quantum interferometry to probe gravity. We obtain the value  $G = 6.67191(99) \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$  with a relative uncertainty of 150 ppm. Our value is at 1.5 combined standard deviations from the current recommended value of the Committee on Data for Science and Technology (CODATA).

**#530 - Optical Lattice Clocks and Applications***Marco Pizzocaro (I) - INRIM**Other Authors: Filippo Bregolin (INRIM, Università di Torino), Michele Gozzelino (INRIM, Università di Firenze), Gianmaria Milani (INRIM, Politecnico di Torino), Benjamin Rauf (INRIM, Politecnico di Torino), Pierre Thoumany (INRIM) Giovanni Antonio Costanzo (INRIM, Politecnico di Torino), Filippo Levi (INRIM), Davide Calonico (INRIM)*

Research on optical frequency standards based on cold atoms or ions has shown a great advance in the last few years. Among others, alkaline-earth atoms trapped in an optical lattice have demonstrated unprecedented stability. Recently a strontium lattice clock demonstrated an uncertainty at the level of  $10 \times 10^{-18}$ , the best in frequency standards up to date.

The stability and accuracy of optical frequency standards will benefit many applications and innovations, such as realization and dissemination of units in the Système International (SI), quantum simulations, relativistic geodesy, test of fundamental constants variation and tests of fundamental physics.

I will describe the development of an optical lattice clock based on ytterbium atoms at the Italian National Metrology Institute (INRIM) and the perspective for the near future.

I will describe the generation of all the laser sources, the physic package and the operation of the clock as well as the experiments in which it is involved.

Comparison with other clocks is planned, both local and remote, that will allow a proof-of-principle relativistic geodesy experiment.

**#531 - THE INRIM - INFN RING LASER GYROSCOPE FOR PLANAR ANGLE METROLOGY APPLICATIONS***Nicolò Beverini - Università di Pisa**Other Authors: J. Belfi, A. Di Virgilio (INFN- sez. di Pisa); M. Astrua, M. Pisani, M. Santiano (INRIM); G. Carelli, E. Maccioni (Univ. di Pisa, dip. Fisica); A. Ortolan (INFN, Laboratori nazionali di Legnaro)*

Ring lasers gyroscopes exploit the Sagnac effect for providing inertial measurements of rotation rate. The rotational motion of their reference frame determines a differential frequency shift (Sagnac frequency) between the two oppositely travelling beams generated inside the optical cavity. In a ring laser of area vector  $A$ , perimeter  $P$  and wavelength  $\lambda$ , this frequency is  $f = 4/(P \lambda) A \cdot \Omega$ , being  $\Omega$  the angular velocity of the cavity frame. Laser gyroscopes with side-length of tens of centimeters are commonly used for inertial navigation applications while larger systems (side-length larger than one meter), rigidly fixed to the ground, provide precise

measurements of the Earth rotation rate and of the small superimposed local rotations coming from geophysical and geodetic phenomena.

Applications of RLGs in Angular Metrology have been foreseen since the end '60s. The basic idea is to use the interference fringes by the two counterpropagating modes as an ultra-fine angular scale dividing the full angle into a number  $N=P/l$  intervals. The most effective realization of such kind of goniometer is the ring laser developed by Yu. V. Filatov and collaborators since the end of 70s, consisting in a monolithic cavity 11 cm in side-length equipped with total reflection prisms in optical contact with a zerodur cavity frame. The typical resolution of these systems is at the level of 100 nrad, typically limited by the errors due to the influence of environmental parameters on the ring laser dynamics.

In a collaboration between INRIM and INFN, we are presently building a new kind of laser goniometer with a target accuracy is 10 nrad, being the accuracy of the most precise angular encoders at the level of some 100 nrad. Our project foresees a square non-monolithic cavity of 0.5 m in side, making use of the last generation dielectric super-mirrors employed in the larger gyroscopes for geodetic and geophysical applications.

We will discuss the main issues and proposed strategies concerning the implementation of an extremely accurate transportable rotational standard, the realization of a very sensitive gyroscope for the measurement of seismic effects, the demonstration of a self-calibration concept leading to the design of a larger rotating RLG for geodetic and relativistic experiments.

### #532 - Doppler-broadened dual-laser absorption spectroscopy for thermodynamic temperature measurements

Livio Gianfrani - Second University of Naples

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The expression of the Doppler width of a spectral line, valid for a gaseous sample at the thermodynamic equilibrium, represents a powerful tool to link the thermodynamic temperature to an optical frequency. This is the basis of a relatively new method of primary gas thermometry, known as Doppler broadening thermometry (DBT). Implemented at the Second University of Naples on  $H_2^{18}O$  molecules at the temperature of the triple point of water, this method recently allowed to determine the Boltzmann constant with a global uncertainty of 24 parts in  $10^6$  [1]. This is the best result ever obtained by using an optical method.

In order to contribute to the new definition of unit kelvin, but also for being useful as a tool for  $T-T_{90}$  measurements, DBT has to approach the target accuracy of 1 part per million (ppm). This talk will resume recent efforts performed in Naples to further develop and optimize DBT. The molecular targets of interest are  $H_2^{18}O$  and  $C_2H_2$ , both showing relatively strong combination vibrational bands at 1.39  $\mu m$ . Main progresses and current limitations will be highlighted. It will be shown that the achievement of the ppm-level is a realistic possibility for the DBT methodology.

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### #533 - Accurate temperature measurements and primary thermometry methods in the determination of the Boltzmann's constant for the new definition of the kelvin"

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By publishing its decision CIPM/103-30, as result of the 103<sup>rd</sup> meeting of 10 December 2014, the CIPM [1] set the deadline of 1<sup>st</sup> July 2017 for submission of experimental data which will lead to the fixed values of the fundamental constants, defining the units of the new SI [2]. When accomplished, the resolution 1 (2011) of the CGPM [3], "On the possible future revision of the International System of Units, the SI", will link the unit of temperature, the kelvin, to a fixed value of the Boltzmann constant  $k_B$ , as also expressed by the BIPM CCU [4] recommendation to the CIPM, U 1 (2013). In its XXVII meeting, in 2014, the CCT [5] identified the most promising methods for the determination of  $k_B$  to be the acoustic gas thermometry, dielectric constant gas thermometry, Doppler broadening thermometry, and Johnson noise thermometry. The methods are based on independent physical principles and very different experimental apparatuses, involving different thermodynamic measurements. At the same time, those methods all have in common the requirements of accurate temperature measurements, and the need that temperature at which measurements are performed is that of the present kelvin definition, being it the triple point of water temperature of 0.01 °C. To improve the present definition, the target relative standard uncertainty of the adjusted value of  $k_B$  must be  $u_{k_B} \leq 1 \cdot 10^{-6}$ . According to the different thermodynamic relationships linking the Boltzmann's constant to the temperature, this objective can be achieved only if temperature measurements are performed, in all the experiments, at maximum with uncertainty of parts in  $10^7$ . In the last years, specific techniques of primary temperature metrology have been defined, discussed and applied to the running experiments, involving standard thermometers made for the purpose, dedicated calibration procedures and special techniques and apparatuses. Such techniques, once established, will be also of fundamental importance to transfer the future new definition of the kelvin backward to the practical scale. This paper reports the most accurate techniques of temperature measurements and controls, developed by the Italian National Institute of Metrology and by Second University of Naples, to achieve the requested target uncertainty for the determination of the Boltzmann constant, during this delicate transition towards a new definition of the temperature unit.

[1]Comité international des poids et mesures - the International Committee for Weights and Measures

[2]International System of Units

[3]Conférence générale des poids et mesures - the General Conference for Weights and Measures

[4]Comité consultatif des unités - [Consultative Committee for Units](#)

[5]Comité Consultatif de Thermométrie - [Consultative Committee for Thermometry](#)

### #534 - The national standards of electrical impedance, in the framework of the new International System of units (SI)

*Luca Callegaro - INRIM - Istituto Nazionale di Ricerca Metrologica*

*Other Authors: Massimo Ortolano (Politecnico di Torino)*

The forthcoming of the new International System of Units (SI), proposed for adoption in 2018, will link the definition of the electrical units to the fundamental constants  $h$  and  $e$ . The Working Group on the SI of the Consultative Committee on Electricity and Magnetism (CCEM-WGSI) has already drafted a set of *Mise en Pratique* for the ampere and the other SI electrical units, including those of resistance and impedance quantities: the ohm, henry and farad.

The ohm, henry and farad can be realized by means of the quantum Hall effect (QHE). Its resistance, a simple submultiple of the von Klitzing constant  $R_K = h/e^2$ , will have an exact value in the new SI. QHE experiments have been employed in National Metrology Institutes since many years. However, the implementation of the traceability chain to derive traceable measurements of resistance, capacitance and inductance at values (often decadic) suitable for dissemination, and the calibration of impedances having arbitrary values, remains a challenge.

The Istituto Nazionale di Ricerca Metrologica (INRIM) is actively pursuing research on the development of devices, measurement methods and dissemination strategies of impedance units that conjugate the accuracy requirements with sustainability in terms of device and labour costs. The talk will focus on:

a) the design of quantum Hall array resistance standards, integrated circuits including quantum Hall elements that provide decadic resistance values with minimal circuit complexity. The circuits are being realized by the National Institute of Metrology (NIM, China);

b) the development of digital bridges for the comparison of impedance standards having ratios in the complex plane. These bridges allow the traceability of impedances having arbitrary magnitudes and phase angles from the practical realization with the quantum Hall effect. The activity is framed within the European Metrology Research Programme (EMRP) Joint Research Project "Automated Impedance Metrology extending the Quantum Toolbox for electricity"; a follow-up is being proposed for the direct realization of the capacitance scale from the quantum Hall effect in novel devices (graphene).

**#535 - A plasmonic fiber-optic nanoprobe for sensitive detection of cancer biomarkers**

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The general demand for effective biological sensors able to efficiently and selectively detect cancer biomarkers is continuously increasing. Moreover, applications such as in vivo biosensing and point-of-care diagnostic require a miniaturized probe performing measurements at precise locations that are often hard to achieve. In this scenario, the integration onto the optical fiber tip of nanostructures supporting localized surface plasmon resonance (LSPR) provides new options to perform remote label-free biological sensing<sup>1</sup>. The light-matter interaction on the fiber surface is achieved through the integration of thin layers of nanostructures supporting resonant modes, highly sensitive to local modifications of the surrounding environment such as molecular binding events. In addition to low sample volumes, other advantages are: real-time detection and simple optical interrogation set-up which, through the small cross-section of the fiber, provide an inherently light-coupled substrate uniquely suited to remote, in vivo and in situ applications. In this work we report a miniaturized LSPR-coupled fiber-optic nanoprobe as a biosensor that is capable of label-free, real time sensitive detection of thyroid carcinomas biomarkers. The device is based on a gold nanostructure supporting LSPR directly fabricated on the fiber tip by means of electron beam lithography and lift-off process. Following a suitable chemical and biological functionalization of the sensing area, human Thyroglobulin has been detected at nanomolar concentrations in biological fluids using as capturing probe a highly specific anti-Thyroglobulin monoclonal antibody. 1. M. Consales A. Ricciardi, A. Crescitelli, E. Esposito, A. Cutolo, A. Cusano, "Lab on Fiber Technology: Towards Multifunctional Optical Nanoprobes,". ACS Nano, 6, 4, 3163–3170, (2012); A. Ricciardi, M. Consales, G. Quero, A. Crescitelli, E. Esposito, A. Cusano, "Versatile Optical Fiber Nanoprobes: From Plasmonic Biosensors to Polarization-Sensitive Devices", ACS Photonics 1, 1, 69–78, (2014)

**#536 - Optical fiber sensors and lab on fiber: Industrial and Medical Applications**

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Optical fiber sensors and lab on fiber: Industrial and Medical applications

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**SUMMARY**

The tremendous decrease of the price of optical fibers early in the eighties of last century has led to a rapid increase of their industrial applications with particular reference to the field of optical fiber sensors. The parallel development of both new materials and nanotechnologies has opened up the road to a large variety of new devices, hard only to think until a few years ago. Taking advantage on this special combination, we have recently developed many different sensors in areas very far away from each other running from railway safety to high energy accelerators, from under water acoustic detection to medical applications. One of the most important emerging results is the lab on fiber, a cousin of the lab on chip, but built on the point of an optical fiber. The small dimensions, the low costs and the absence of electrical wires in the measurement area is leading towards a powerful multiparametric device for medical in vivo diagnostics: the sensorized needle.

Accordingly, this paper is organized as follows. After a brief introduction of both the basic technology and the lab on fiber concept we describe a large set of applications, we have realized so far. They range from a system to measure the weight of a train together with the detection of tire defects to an under water four element acoustic antenna with beam forming as well, from simultaneous measurements of strain, temperature humidity and magnetic fields in high energy accelerators at cryogenic temperature to a sensorized needle for either in vivo cancer markers detection or for high efficiency loco regional anesthesia.

**#537 - Whispering-gallery mode resonators based on liquid droplets**

*Gianluca Gagliardi (I) - CNR, Istituto Nazionale di Ottica (INO)*

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Over the last decade, optical whispering-gallery modes (WGMs) have been observed in solid micro-cavities of various geometries. WGMs supported by dielectric microspheres and toroids exhibit an optical field that is confined near to the surface. Using highly-transparent glasses, light that is coupled into a WGM can circulate around the resonator for a long time before being scattered or

absorbed. Q factors  $> 10^9$  can be achieved using silica material. Silica resonators proved ultra-sensitive bio-chemical probes but were also studied as miniature systems to observe coupling and interaction phenomena between light and matter. The peculiarity of WGMs is that light travels along closed paths at the interface between the surface of the resonator and the surrounding environment. Unfortunately, most of the light circulates inside the resonator and only the evanescent wave tail may interact with the external medium, i.e. only a small fraction of light is actually used for sensing, thereby reducing the effective cavity enhancement. Here, we propose to use liquid droplets as micro-resonators for sensing applications. The droplet itself serves as the sensor and the sample at the same time, where the internal optical field is directly used to probe dissolved analytes or particles. We demonstrate free-space excitation and laser frequency locking on whispering-gallery modes in vertically-suspended liquid droplets [1]. Photon lifetime measurements are performed by cavity ring-down techniques recording Q-factors ranging from  $5 \times 10^5$  to  $10^8$  in the near-infrared and visible spectral regions. Lifetime changes are measured in mixtures made from different liquids as a proof-of-concept of chemical sensing. Investigations on Q-factor limitation due to thermally-induced shape fluctuations are performed. Effects of metallic nanoparticles dissolved in the droplets were studied in view of possible plasmon-assisted detection of rare analytes [2]. Appealing applications for spectroscopy, biosensing, material characterization and cavity opto-mechanics are envisaged.

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- 2) M.R. Foreman, S. Avino, R. Zullo, H.-P. Looock, F. Vollmer, and G. Gagliardi, *Eur. Phys. J. ST* 223, 1971 (2014)

### #538 - Dispersive shock waves: from water waves to optical fibers

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Dispersive shock waves are a fascinating phenomenon that occurs in non-dissipative media that exhibits weak dispersion and strong nonlinearity, with the latter inducing a propagating wavepacket to develop a steep front (shock wave), which is subsequently regularized by the onset of fast spontaneous oscillations which fill an expanding region in space and time. We present experimental evidence for this phenomenon in two complete different settings. The first is concerned with the propagation of a modulated laser field in an optical fiber. In this case the optical field breaks around the point of zero (or minimum) intensity giving rise to an expanding fan of oscillations made of dark soliton-like excitations. In Fourier space this is accompanied by the generation of a huge cascade of sidebands of the input modulation frequency via multiple four-photon processes. In the second setting we have studied the propagation of a controlled water wave disturbance propagating in a tank in the regime of shallow water. The breaking of the initial disturbance and the appearance of the dispersive shock is successfully monitored along the tank.

We show that these two apparently diverse phenomena have a common origin in terms of the regularization of classical shock waves which occurs in the regime of weak dispersion.

Both can be modeled by weakly dispersing nonlinear partial differential equations (the well known nonlinear Schrödinger equation and the Korteweg De Vries equation, respectively). In particular the fiber experiment can be described in terms of equivalent hydrodynamic variables as well as Whitham modulation approach, revealing that the light field exhibits properties of a photon fluid that mimic those of a real fluid.

### #539 - Tri-axial FBG strain sensor for volcano monitoring

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Fiber Bragg Grating (FBG) sensors are nowadays an extensive tool for monitoring, diagnostics and control in civil engineering. However very limited literature exists on geophysical applications of FBG sensors, although these devices might have a potential impact in such field.

We developed an FBG strain sensor specifically designed for volcano monitoring; i.e. with special care to trade-offs among resolution, power consumption, and cost. The system features significantly higher resolution and accuracy in static measurements with respect to previous implementations of the FBG technology to study rock deformations. Moreover, the sensor has been developed in tri-axial configuration.

A field campaign was carried out with a preliminary single-axis FBG strain sensor prototype on Mt. Etna, in order to check the system performances in out-of-the-lab conditions and in the hostile volcanic environment (lack of mains electricity for power, strong diurnal temperature changes, strong wind, erosive ash, snow and ice during the winter time), and to determine whether measurable changes are induced across a 1989 fracture system during the paroxysmal phases of Etna's volcanic activity. We found positive correlations between the signal detected by the FBG strain meter and the volcanic tremor detected by a seismic station at Mt. Etna (ESPC). This represented an encouraging result since the installation has been performed on a surface trace where the signal is dominated by thermally induced strain, whereas the final prototype will be installed underground thus the sensitivity of the device to micro tremors will increase.



**#540 - Coupled-resonator sensors: beyond the standard cavity enhancement.**

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In all radiation-matter interaction applications, the use of an external cavity to extend the interaction length is common. Within the intracavity path, the probability of interaction is in fact multiplied by a factor proportional to the cavity finesse. The effective equivalent interaction pathlength achievable with a cavity is thus only limited by the quality factor of the resonator and by the excess noise associated with the cavity injection: with a sufficiently high finesse cavity and a low-noise detection scheme the interaction probability can be increased by several orders of magnitude.

In this work we demonstrate that the pathlength enhancement of a Fabry-Perot cavity can be increased beyond the limit set by its quality factor by exploiting the modal interference occurring in a coupled resonant system. The system considered in this work is formed by a Fabry-Perot (FP) cavity enclosed within a larger ring resonator. We show that the FP intracavity losses have a deep impact on the nature of the resonant system itself. For example, at zero losses, when the internal FP is impedance-matched the system reduces to a simple ring resonator. As the FP losses increase, its transmission vanishes and the system slowly turns into a standing-wave resonator. The metamorphoses of the resonant spectrum that accompany the described transitions give rise to a series of interesting phenomena, such as ultrasensitive extinction, transparency and reversed extinction of the coupled-resonator modes. These phenomena are experimentally observed in a Fabry Perot fiber resonator enclosed in a fiber loop, and described theoretically by means of an intuitive analytic model. The ultrasensitive extinction regime, particularly attractive for all the radiation-matter interaction experiments, is object of a more quantitative investigation. The equivalent interaction pathlength of the presented resonator are directly compared with that achievable with a traditional cavity by recording the transmission of the internal Fabry-Perot for different loss levels in both open-loop and closed-loop configuration. In the latter situation, the coupled resonator modes show a sensitivity to the intracavity losses 10 times larger than the modes of the equivalent standalone FP resonator. The results are consistent with the predictions of the theoretical model, and demonstrate for the first time that the absorption sensitivity of a Fabry Perot resonator can be improved largely beyond the limit imposed by its quality factor.

**#541 - Engineered LSPR nanosensors based on Photonic Quasi-Crystals for Environmental analysis**

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The progress of the nanotechnology in the last years has made possible to realize tailorable artificial structures for the control of the light in many applications in the photonic field. An example of artificial electromagnetic (EM) materials are the metamaterials (MTMs) as photonic crystals (PCs) and the photonic quasi crystals (PQCs), which are very attractive given that they allow new possibilities to control the EM field in innovative ways. With the use of these classes of materials, it is possible to realize novel optical sensing devices based on the extraordinary plasmonic properties of noble metal nanoparticles characterized by selective EM responses, which undergo significant frequency shifts, in presence of a specific target molecule. Various plasmonic sensors based on nanotechnology have been recently developed for the sensing of low concentrations of molecules of biological or environmental interest. Among them Localized Surface Plasmon Resonance (LSPR) based nanosensors are considered one of the most powerful tools in the biotechnology and sensor fields. They operate transducing small changes in refractive index near the metallic surface into a measurable wavelength shift response and they have the following notable advantages: high sensitivity, good reproducibility, label-free detection, low cost and easy instrumental setup.

In the present work we engineered reproducible LSPR nanosensors based on gold PQCs patterns realized with different geometries. We use the Electron Beam Lithography (EBL) for the fabrication of these nanosensors. The EBL system permit to control with high precision size, shape, but also the inter-particle distance and consequently to tune the plasmonic resonance of the nano-arrays in the visible and near infrared range. The sensitivity of the nanosensors has been evaluated and high values ranging from 210 to 270 nm/RIU have been obtained for a-periodic patterns with different shapes of the nanoparticles. The performance of the LSPR nanosensors for environmental analysis has been tested using a pesticide (Thiram, C<sub>6</sub>H<sub>12</sub>N<sub>2</sub>S<sub>4</sub>) at different concentrations. A limit of detection of the order of nM has been obtained using a LSPR nanosensor based on a Thue-Morse pattern. These first results indicated that the LSPR nanosensors developed are expected to demonstrate a wide range of applications for the detection of analytes of environmental and biological interest.

**#542 - Phosphorene, a new two dimensional platform for advanced materials**

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Two dimensional materials are still an unexplored territory. Graphene is one of the principal platform on which material scientists have only recently started to play.[1] On the other side, it was estimated that a few hundreds of layered materials could be exfoliated to give a 2D crystal, allowing a large growing opportunity of research.

Only small amounts of single and few layers sheets of Phosphorene, the all-P counterpart of graphene, have been prepared by exfoliation of black phosphorus, the most stable and least reactive of the allotropic forms of phosphorus, either by micromechanical cleavage (Scotch tape method) or liquid exfoliation.[2]

A phosphorene sheet has the same honeycomb hexagonal network of graphene but it is corrugated having the P atoms an  $sp^3$  hybridization. Phosphorene is a natural semiconductor, and the band gap can be controlled by changing the number of stacked layers. This makes the materials very promising for a wide variety of electronic applications.

On the other hand, almost nothing is known about the reactivity and the physico-chemical properties of this new fascinating material, and only sparse theoretical [3] and experimental [4] studies have been reported so far.

In this communication, we present our results on the synthesis of phosphorene. We will describe its adsorption properties towards different gaseous molecules, such as  $CO_2$ , CO,  $O_2$  and  $H_2$  and its functionalization using metallic fragments or metal nanoparticles.

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**#543 - Multilayered Ge quantum dots embedded in SiO<sub>2</sub>: structural and optical analysis**

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In the past years Ge quantum dots (QDs) gained a renewed scientific interest over Si QDs due to the lower synthesis temperature, higher absorption coefficient and larger exciton Bohr radius [1]. The optical behavior and the band-gap tuning of Ge QDs do not simply depend on the size, as the quantum confinement effect (QCE) predicts, but also on QD-QD distance and ordering. In this work, Ge quantum dots (2-10 nm in diameter) in SiO<sub>2</sub> grown by plasma-enhanced chemical vapor deposition, will be reviewed evidencing whether and to which extent the quantum confinement affects the light-matter interaction. In order to investigate the features of QCE by controlling the QD diameter, multilayers of Ge QDs embedded in SiO<sub>2</sub>, separated by an SiO<sub>2</sub> barrier layers (20 nm thick) were synthesized by plasma enhanced chemical vapor deposition and annealing at 800°C. The multilayer approach allows a narrower size distribution in comparison to single layer of QDs (where no SiO<sub>2</sub> barrier layers are involved). We present a detailed study on structural and optical properties of multilayer samples compared with single layer ones. In multilayer samples TEM analysis shows a narrow size distribution of very small Ge QDs (~2 nm). Using UV-Vis-NIR spectrometry and Tauc analysis of the absorption spectra, the optical bandgap and the absorption efficiency of Ge QDs were extracted. In comparison to single layer samples, with similar optical band gap values (~1.8±0.2 eV), multilayered Ge QDs show a light absorption efficiency ten times higher. This effect evidence that a significant QD-QD interactions exists which greatly affect the light absorption efficiency.

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**#544 - Phosphorus Diffusion and Incorporation in Silicon Nanoclusters Embedded in Silicon Oxide**

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Doping has a crucial role in tailoring optical and electronic properties of semiconductor nanostructures. The study of impurity incorporation processes is therefore an important part of the know-how needed to design future devices, more in detail, deterministic doping of nanostructures requires the knowledge of the interface atomic transport thermodynamics at the nanoscale. Our contribute to this hot topic was to approached the problem at the extreme case of 3D nanoscale confinement by studying the P incorporation of Si nanocluster (NCs) embedded in SiO<sub>2</sub> matrix. Previous experiments demonstrated that P is trapped inside the clusters when P incorporation occurs simultaneously with the NCs formation. In this work we adopted an innovative method: we induced the incorporation by diffusion of P from a spatially separated solid source on still formed and stable NCs.

The performed experiment allows for a quantification of the P content in NCs and demonstrates that P traps within Si NCs (not at oxide interface), with a concentration 6 times above the solid solubility in bulk Si. Combining advanced material synthesis, multi-technique experimental quantification, and simulations of diffusion profiles with a rate-equation model, we experimentally estimated the energy barriers for P diffusion in SiO<sub>2</sub> and trapping/de-trapping at the SiO<sub>2</sub>/Si NCs interface, and provide a decisive description of the system very close to equilibrium. A binding energy of 1eV is measured indicating that trapping is thermodynamically favored and not only kinetically favored by Si phase transitions occurring during doping. We compared the estimated P binding energy to Si NCs with several existing ab-initio calculations, indicating a strong role of dangling bonds at the Si/SiO<sub>2</sub> interface in the dopant trapping/de-trapping mechanisms.

Incorporation of high concentration of dopant impurity in small crystals is an intriguing possibility that may open the route to a diffusion-controlled doping of Si nanostructures. We have started to investigate this diffusion doping method in combination with monolayer contact doping that can provide a controlled source of dopant conformally distributed on 3D structures very appealing for future devices processing.

#### #545 - Synthesis, optical properties and in situ doping of freestanding Si nanoparticles

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Nowadays, the synthesis of nanostructures seems to be an appealing way to overcome the intrinsic limit in scaling down of electronic devices as it offers the possibility to obtain single crystal electronic device. In this sense, plasma deposition is an effective way since different nanostructures are possible by controlling plasma conditions. This approach provides also the great advantage to use low cost substrate.

Nevertheless, the capability to control the optical and electronic properties of such nanomaterials is still an open issue. Precise control on size distribution and shape of plasma deposited nanostructures is not trivial as well as introducing dopant species.

We have obtained single-crystal silicon nanoparticles (Si-NP) by using inductive coupled plasma (ICP) CVD. At a substrate temperature not exceeding 50°C, it was possible to have mono-dispersed size distributions in the range between 10 and 200 nm. Si-NP are spherical up to 20 nm in diameter. Above this size, the Si-NP are characterized by an octahedral shape faced along well-defined crystalline planes, mainly {111}. On isolated Si-NP light trapping effect was probed by an enormous amplification of Raman peak up to 10<sup>8</sup> times the value of a similar bulk Si volume. The mechanism conceived and optimised for obtaining such a result was related to the capability of a Si octahedron to trap the light because of its geometrical parameters. Moreover, thanks to the flat surfaces of the octahedra, Si-NPs produce a very efficient light scattering effect for the non-trapped portion of impinging light. Furthermore, we also synthesized in situ n-doped Si-NP using phosphine as precursor gases. The doped particles, nucleated and grown in plasma, are still octahedra but surrounded by a defective shell. Thanks to geometrical interpretation of the chemical profile was possible to understand the spatial distribution of phosphorus which is essentially confined at the surface. Here, its concentration is around 1 %. Thanks to scanning capacitance microscopy technique we observed that phosphorus is electrically active in both octahedral and spherical particles.

Having control of size, shape and doping of nanostructures represent a significative step towards a wide integration of plasma based nanostructures in photonics and photovoltaic applications.

#### #546 - Energy recycling under conditions of phonon and electron confinement

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Ensembles of silicon nanocrystals (Si NCs) are widely investigated for their interesting properties and applications in optoelectronics and photovoltaics. The phenomenon of photoluminescence (PL) saturation appears in these materials due to Auger recombination of multiple excitons located in the same NC, setting an upper limit for the photovoltaic conversion efficiency<sup>1</sup>. Here, we present dedicated investigations of PL saturation for thin layers of Si NCs in an SiO<sub>2</sub> matrix. In contrast to the established standard picture, we reveal a persistent increase of PL intensity above the saturation point. We thoroughly investigate the PL characteristics in and beyond the saturation regime over an irradiance range of more than four orders of magnitude, for samples with different average

Si NCs sizes and concentrations. We conclude that complete saturation cannot be achieved even for the highest available irradiance, with the PL intensity continuously increasing, albeit at a different (lower) rate. Experimental artifacts are excluded as a possible reason for the observed behavior. We explain the experimental findings with a theoretical model taking into account the massive electron-hole pair production per single NC and the confinement of phonons and electrons in the NC, resulting in more emitted photons than expected according to the established standard picture. An alternative model, taking into account reduction of Auger recombination of the biexciton<sup>2</sup>, is also considered, but found less credible. These results offer better insight into the mechanisms of energy conversion and dissipation in ensembles of Si NCs in solid matrices, and open novel avenues for efficiency increase in future photovoltaics, among others.

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#### #547 - Stacking sequence characterization of GeSbTe grown on Si(111) by Molecular Beam Epitaxy

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Phase-Change Materials (PCMs), mainly represented by GeTe-Sb<sub>2</sub>Te<sub>3</sub> (GST) alloys, are used for high-density data storage in optical media and for solid-state non volatile memory [1]. Recently, it has been shown that multi-layered crystalline phase change memories, such as interfacial PCM (iPCM) can have improved functional properties [2], indicating that the crystalline growth of phase change materials is a viable approach for device fabrication. Molecular Beam Epitaxy (MBE) has been successfully used to fabricate epitaxial phase change materials, making advanced studies on the properties of these materials possible [3]. High Angular Annular Dark Field (HAADF) Scanning Transmission Electron Microscopy (STEM) directly relates the micrograph contrast to the atomic number (Z-contrast), permitting a straightforward interpretation of the images. Through this characterization technique here we provide a complete analysis of the MBE GST film investigated.

Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> films were grown epitaxially on a Si(111)-(√3 × √3) R30°-Sb surface at 250 °C, in a molecular beam epitaxy (MBE) chamber equipped with separate Ge, Sb, and Te effusion cells. The sample thickness was 100 nm. Films were capped with 30 nm thick layer of amorphous ZnS-SiO<sub>2</sub> to inhibit oxidation due to air exposure [4-5]. A JEOL ARM200F Cold FEG STEM/TEM with a resolution of 0.68 Å, working at 200 kV, was adopted to obtain HR micrographs of the sample. The film was observed in the [110] zone axis, containing the c-axis direction, in order to directly observe the stacking sequence of the atomic planes along it.

By HAADF STEM analysis we clearly distinguished the stacking sequences, formed by 7, 9 or 11 planes, corresponding to Ge<sub>7</sub>Sb<sub>2</sub>Te<sub>4</sub>, Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> and Ge<sub>3</sub>Sb<sub>2</sub>Te<sub>6</sub>, respectively. In particular, van der Waals (vdW) gaps were clearly observed between two Te planes [6], as indicated by the most strong Z-contrast signal.

The less intense planes exhibited almost the same value, indicating that Ge and Sb are uniformly distributed in the same lattice site, accordingly to the structure proposed by Matsunaga *et al.* [6].

Along the stacking sequence, for all the stoichiometries, different plane spacing was clearly distinguished. The spacial width of the vdW gap amounts to 2.7 Å, the planes adjacent to vdW gap are characterized by a spacing of 1.6 Å, while the next plane lies at a distance of 2.1 Å. This difference might be associated to the strength of the bonds Te-Te (vdW gap) and Te-Ge/Sb.

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#### #548 - Photoluminescence Emission from a Scanning Probe Tip Made of Epitaxial Germanium

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Detecting single molecules with high sensitivity and molecular specificity is of great scientific and practical interest in many fields such as chemistry, biology, pharmacology and environmental science [1]. The absorption of light by a molecule depends on the intensity of the local electric field. The near-field coupling of electromagnetic light waves to single selectable nano-objects is the most promising approach to achieve sub-wavelength spatial resolution. This work shows the progress towards single-molecule identification by demonstrating photoluminescent (PL) emission from a scanning probe tip made of epitaxial semiconductor material.

Specifically, the tip design and fabrication of in the form of a 1  $\mu\text{m}$  tall epitaxial germanium pyramid was conceived for 3-dimensional (3-D) mid-infrared antennas to be used as plasmonic field concentrators for scanning near-field infrared microscopy (s-SNIM). Epitaxial germanium was grown on a silicon substrate by low energy plasma enhanced chemical vapour deposition. Pillars of circular shape, 1  $\mu\text{m}$  diameter and aspect ratio of 6 were fabricated by electron-beam lithography and deep reactive-ion etching. The top 2  $\mu\text{m}$  are made of heavily doped Ge. The tip of an atomic force microscopy (AFM) cantilever is glued to the top of the pillar and the patterned SiGe structures are then released by focused ion-beam (FIB) milling of the pillar base. The final shaping of the pyramid is also done by FIB milling [2]. The AFM cantilever with the Ge tip was then mounted in a s-SNIM setup (by Neaspec GmbH, experiments are reported elsewhere). One of the tips was instead mounted in a confocal micro-PL emission setup, where the illumination wavelength of 1060 nm excites electron-hole pairs in the Ge tip that subsequently recombine at the direct gap energy gap of Ge (0.86 eV, 1550 nm). The PL emission was dispersed in a home-made spectrometer working in the NIR range (800-1700nm) and detected via an InGaAs avalanche diode while scanning the tip in the focal point of both the detector and the illumination beam. A strong and tightly-confined emission was recorded from the tip apex. The micro-PL spectrum of one of the pillars not used for tip fabrication was also measured in the same setup. The spectral shape of the emission, peaking around 1550 nm, closely resembles the emission of the pillar right before the fabrication process indicating that the optical properties of the material in this wavelength range were preserved during the FIB milling process.

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#### #549 - Locally tensile-strained Ge induced by nanopatterning of epitaxial SiGe

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Strain engineering in semiconductors can be used to control their critical properties. A 4% uniaxial tensile strain, applied along the [100] direction, would transform Ge into a direct band gap semiconductor. If achieved, its compatibility with Si-based technology would make it ideal for many microelectronics and optoelectronics applications[1]. In this work, top-down SiGe nanostructures are used as stressors for the creation of high deformation fields in Ge(001) [2,3].

On top of a Si(001) substrate, a strained  $\text{Si}_{0.5}\text{Ge}_{0.5}$  film is grown on a Ge relaxed buffer by low-energy plasma-enhanced chemical vapor deposition (LEPECVD), and x-ray diffraction (XRD) is performed in order to verify the composition and the strain state of the as-grown heterolayers. Afterwards, electron-beam lithography (EBL) and reactive ion etching (RIE) are used to pattern the SiGe layer into parallel stripes, in order to exploit the perimetral forces they exert to obtain tensile-Ge in the gaps between them. The pattern design was modeled by finite element method simulations (FEM), while the induced strain levels are inferred by micro-Raman spectroscopy.

We have found that the Ge peak is shifted to lower wavenumbers (which means higher tensile strain) as the gap between stripes is reduced. The extracted strain values are in good agreement with the FEM simulations. Furthermore, the detected strain for a 20nm gap is beyond the critical value for the indirect to direct gap transition[4].

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#### #550 - Strain release management in SiGe/Si films by substrate patterning

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The random nucleation of misfit dislocations associated with the plastic relaxation of Si-rich SiGe epilayers on Si hinders the possibility to use them in several applications, for example in photodetectors [1]. In the present work we demonstrate that through the use of a suitable substrate patterning, it is possible to confine the nucleation and the propagation of misfit segments and threading arms during the epitaxial deposition of  $\text{Si}_{1-x}\text{Ge}_x$  alloys [2]. This leads to the creation of microns-large coherent areas,

which are free of dislocations. Thick Si-rich  $\text{Si}_{1-x}\text{Ge}_x$  ( $x \sim 10\text{-}20\%$ ) films have been deposited on templates fabricated on Si (001) substrates by electron beam lithography, dry and anisotropic wet-chemical etching. The pattern is composed of a matrix of submicron-sized inverted pyramids along the  $\langle 110 \rangle$  directions on a Si(001) substrate. A systematic study of different parameters (Ge content, film thickness and growth temperature) has been performed to optimize the process [3]. All the samples have been characterized by atomic force microscopy (AFM), verifying that the patterning induces the propagation of bunches of misfit segments just along the pit rows, in the [110] and [1-10] directions. Moreover, the threading arms are mainly trapped in the pits: thus large square areas result to be strained, still dislocation-free. Such a control is not confined only within the pattern, but extends over  $20 \mu\text{m}$  outside it. The strain in the system has been characterized by  $\mu\text{Raman}$  spectroscopy. The results show a full compressive value in the dislocation-free region, while relaxed stripes have been observed above the bunches of misfit. This is the first case where  $\mu\text{Raman}$  spectroscopy has been used for the visualization of the dislocations present in a film. Moreover, diffraction experiments were performed using a nano-focused X-ray beam at the ID01 beamline of the European Synchrotron Radiation Facility in Grenoble. Fast-scanning X-ray nanodiffraction microscopy [4] was used to directly visualize the misfit dislocation network. X-ray real-space diffracted intensity maps have been compared to AFM images. The perfect match between the nano X-ray maps and the AFM analyses confirmed the capability to control the dislocation propagation using a suitable pattern [5]. This system is kinetically stable against thermal treatment, so that fabrication of devices with thermal budget on top of the SiGe strained square-areas should be possible.

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**#551 - Shedding light on 2D materials using synchrotron radiation**

*Silvano Lizzit (I) - Elettra Sincrotrone Trieste*

The rising interest of the scientific community to graphene, the two-dimensional (2D) material composed by carbon atoms arranged in a honeycomb lattice, is motivated by its unique electronic and physical properties which make it one of the most promising materials for future nano-technologies. The scientific community is also dedicating increasing interest in other 2D atomic crystals such as hexagonal boron nitride (h-BN) or transition metal dichalcogenides. Many experimental and theoretical works have been performed, aimed to the synthesis and characterization of 2D materials. A wealth of experimental techniques, based on a surface science approach, have been used to perform these studies.

The talk will be dedicated to synchrotron radiation studies on graphene and other 2D materials (h-BN in particular), using high energy resolution X-ray photoemission spectroscopy (HR-XPS) and photoelectron diffraction (XPD). The XPS technique, used also in its fast modality to follow transient processes (Fast-XPS), and combined with theoretical modeling and complementary surface science techniques, is an extraordinary tool capable of exploring several aspects inherent to the chemistry and physics of materials in general, 2D atomic crystals in this specific case. The presentation should highlight the use and the information content obtained by exploiting these techniques. The presented topics will cover from the growth of graphene and h-BN on metal substrates, to the study of their electronic, structural and chemical properties.

**#552 - Ultrafast dynamics and transient electronic states in complex materials**

*Marino Marsi (I) - Université Paris-Sud*

Ultrafast dynamics and transient electronic states in complex materials

M. Marsi

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The development of femtosecond light sources opened new perspectives in terms of manipulating the properties of condensed matter over ultrafast time scales. On one hand, they represent a novel method to explore the properties of complex materials, alternative and complementary to more traditional experimental techniques; on the other hand, they disclosed the possibility of changing the properties of matter using light pulses, and of creating transient electronic and structural phases that cannot be reached changing conventional thermodynamic parameters like pressure, temperature or chemical doping.

The combination of ultrafast spectroscopies using different wavelengths from the optical domain to the X-rays can be crucial for our understanding of these photoexcited states of matter: time and angle resolved photoelectron spectroscopy, in particular, can provide a direct visualisation of transient electronic states in reciprocal space, as demonstrated by the recently commissioned FemtoARPES setup [1]. Selected examples will be discussed to illustrate these possibilities in the study of Mott materials and topological insulators [2,3].

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**#553 - Status of the STAR Project at UniCal**

*Luca Serafini (I) - INFN-Milan*

The STAR Project is in progress at the University of Calabria (UniCal) in the frame of the PON Materia initiative. Based on a collaboration among UniCal, CNISM, INFN and ST, it comprises the construction of a Thomson back-scattering X-ray source for applied research. The installation of main machine components (RF laser-driven photo-injector, collision laser system, beam lines, control system and diagnostics) has just started, with perspectives to begin the machine commissioning in mid 2016. We will present the advancement status as well as future plans for machine upgrade that are being prepared in the context of the PON-2020 calls for proposal for research infrastructure upgrades.

**#554 - Attenuation length of low energy electrons in solids**

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The measurement of the information depth of electron spectroscopies for different materials and different energies is of great interest. Several studies have already shown that the "universal curve" of the electron mean free path is not universally valid and can strongly depend on the material [1]. In particular, this issue is relevant for systems featuring surface properties different from

bulk ones, like correlated materials, buried interfaces and capped samples. Specifically, bulk sensitivity at very low energy (less than 10eV) is still an open question [2].

In this work we have determined by the over-layer method the effective attenuation length (EAL) of electrons in the (6-28) eV energy range for MgO films. By correlating measurements with the band structure of the material, the energy dependence of the EAL can to a good approximation be explained by the joint density of (occupied and unoccupied) electronic states of MgO. Similarities and differences with respect to the corresponding results on CoO (a smaller gap - insulator) and Yb films are discussed [3, 4]. Comparison of experimental findings on MgO with optical properties calculations available in literature suggests that, for energies lower than 20 eV, the scattering mechanism are described by the imaginary part of the dielectric function, accounting in particular for the steep increase of the EAL for energies lower than the insulator band gap.

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### #555 - Probing Long-Lived Plasmonic-Generated Charges in TiO<sub>2</sub>/Au by High-Resolution X-ray Absorption Spectroscopy

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Exploiting plasmonic Au nanoparticles to sensitize TiO<sub>2</sub> to visible light is a widely employed route to produce efficient photocatalysts. However, a description of the atomic and electronic structure of the semiconductor sites in which charges are injected is still not available. Such a description is of great importance in understanding the underlying physical mechanisms and to improve the design of catalysts with enhanced photoactivity. We investigated changes in the local electronic structure of Ti in pure and N-doped nanostructured TiO<sub>2</sub> loaded with Au nanoparticles during continuous selective excitation of the Au localized surface plasmon resonance with X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS). Spectral variations strongly support the presence of long-lived charges localized on Ti states at the semiconductor surface, giving rise to new laser-induced lowcoordinated Ti sites.

These results have been published in *Angew. Chem. Int. Ed.* 2015, 54, 5413–5416

### #556 - Copper-Phtalocyanine thin film on Al (100) crystal surface: a study of site-projected molecular orbitals through Auger-Photoelectron Coincidence Spectroscopy (APECS)

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Metal-phtalocyanines are organic molecules which present a relatively high mobility and a 1.9 eV energy gap between highest occupied and lowest unoccupied electronic levels.

The interaction of this molecule with a metal substrate is a fundamental aspect to investigate because it can induce changes in electronic structure, condition the orientation of molecules, and also cause long-range ordered growth, with great increase in mobility.

Aluminum is a good example of a strongly-interacting substrate, since it has almost free and highly delocalized *p* conduction electrons. Previous studies of this interface have given evidence of a relevant charge transfer from substrate to molecule at the monolayer stage.

To get more insight in the modification of electronic structure due to the substrate, we have performed Coincidence Spectroscopy measurements between C1s photoelectrons and Auger C KVV electrons, in function of the film thickness. Indeed, Auger electron spectroscopy from KVV lines gives information on the molecular orbitals of a system, and thus on the electrons which are involved in the bond with the substrate. On the other side, C 1s XPS spectrum presents a chemical shift of 1.4 eV between the non-



equivalent carbon atoms, namely the pyrrole-ring carbon and the benzene-ring one, thus giving the possibility to be site-selective. Combining the two information with coincidence measurements, we have an information on the site-projected molecular orbitals of the system.

Our experiment has been performed at ALOISA beamline in ELETTRA synchrotron (Trieste). Our results show a clear shift (ca. 3 eV) of Auger spectrum going from thick film to monolayer for the Al substrate, thus confirming the relevant modification of electronic structure, with charge transfer towards molecule. In particular this shift is more relevant in coincidence spectra with benzene-ring photoelectron, an indication that the transfer involves orbitals localized mostly on benzenic rings.

#### #557 - XANES and EXAFS study of the Fe K-edge in the FeBTC Metal-Organic Framework

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Due to the low toxicity and the high biocompatibility of iron, an increase in the use of iron-based MOFs is widely regarded as a highly desirable target.<sup>1</sup> FeBTC, a metal organic framework commercially known as Basolite F300, is widely available and exhibits high catalytic activity for a large variety of organic transformations.<sup>2</sup> The oxidation state of iron atoms is found to be +3<sup>3</sup> but the local environment around iron is until now unsettled.

In this work we discuss the results of an experimental investigation carried out at the XAFS beamline of ELETTRA Synchrotron. We present the determination of the local environment around the metal ion in FeBTC performed by combining XANES and EXAFS studies of the iron K-edge.<sup>4</sup> XANES spectra point out the prevalence of Fe(III) both in a sample stored in air and in that activated by a dehydration treatment. The ligands around iron are found to be arranged in octahedral geometry. Dehydration induces a change in the coordination of the first shell and a decrease of the d-orbital occupancy after the activation is detectable, while preserving the network. We propose that the local structure around Fe atoms does not undergo a rearrangement upon the activation, thus leading to the formation of an open metal site. The analysis conveys that the FeBTC is a disordered network of locally ordered blocks.

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**#558 - Theoretical core-level spectroscopy from adsorbed organic molecules**

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Hybrid interfaces between organic molecules and inorganic substrates are key systems in many technological applications, ranging from photovoltaics to organic field effect transistors and light emitting devices. Several properties of such interfaces can be effectively studied by electron core-level spectroscopies: X-ray photoemission (XPS) addresses changes in the chemical state of the atoms; near-edge X-ray absorption fine structure (NEXAFS) accesses molecular orientations and provides information on the unoccupied electronic levels; resonant photoemission spectroscopies (RESPES) can measure interfacial electron transfer times down to the femtosecond timescale.

The potential of these experimental techniques is fully obtained by complementing them with theoretical investigations and reliable numerical modeling. The perturbation by charged atomic cores is efficiently taken into account within a density-functional theory (DFT) based approach, as will be exemplified here. Numerical simulation of the dependence of NEXAFS molecular spectra on the photon electric field direction for pentacene and perylene derivatives [1,2] demonstrates how one can completely determine the orientation (polar and azimuthal) of molecules at interfaces. Disentangling the contribution of specific atomic cores (initial states) and molecular orbitals (final states) to NEXAFS [2], is further used to demonstrate filling of the lowest-unoccupied molecular orbital of pentacene in the peculiar V-bent conformation it assumes on Al(001) [3]. Excitonic effects due to the presence of core-excited atoms in the molecule can be included in the modeling to understand the electron-transfer times as measured by RESPES, which are evaluated numerically for molecules on a semi-infinite TiO<sub>2</sub>(110) substrate whose continuum of conduction states is described by Green's function techniques [4].

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**#559 - Chemical characterization of surfaces with spatially resolved photoemission spectromicroscopy: fuel cells, nanosensors and novel materials**

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Due to the short escape depth of electrons, usually less than a few nm, photoelectron spectroscopy is the best surface sensitive analytical technique for probing chemical composition and electronic properties of surfaces and top layers of samples. Nevertheless the standard approach to this technique suffers from two major limitations: 1) spatial resolution (material gap) and 2) the requirement for high-vacuum environment (pressure gap).

The Scanning PhotoEmission Microscope (SPEM) uses a direct approach to add the spatial resolution and characterize chemically surfaces and interfaces at the submicron scale i.e. the use of a small focused X-ray photon probe to illuminate samples. Focusing of X-ray beams is performed by Fresnel lenses (zone plates) while elemental selective maps are obtained by scanning samples with respect to the focused beam. In the SPEM hosted at the ESCAmicroscopy beamline at the Elettra synchrotron light source, the X-ray beam can be downsized to a diameter of 120 nm which allows imaging resolution of less than 50 nm.

The unique properties of photoemission spectroscopy to shed light on the chemical and electronic properties of surfaces offer a powerful tool of analysis for a wide class of scientific and technological topics. The main results obtained by using the SPEM in the characterization of materials used for the fabrications of solid oxide fuel cells, electrochemical devices, nanosensors and materials will be presented aiming to disseminate properties and performance of this novel type of microscopy.

Only recently the development of electron energy analyzers with differentially pumped lens systems allowed to perform in situ XPS measurements up to few mBar (near ambient pressure). Due to their cost, technical complexity and intrinsically low efficiency it was not possible to export such solution to photoemission spectromicroscopy and conventional XPS stations so far. The SPEM hosted at Elettra is now able to offer to the scientific community a new compact near ambient pressure cell allowing in operando spatially resolved XPS characterizations at mBar gas pressures. The first results recently obtained at Elettra will be shown.

**#560 - Bonding and reactivity at catalytic interfaces: Modelling novel fuel-cell electrodes from ideal to realistic reaction environments**

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Platinum-group metals supported and dispersed on highly reducible oxides are common active catalysts for the industrial synthesis of chemical products and for renewable-energy applications such as fuel cells or artificial photosynthesis. Due to the high price of Pt, the sustainable development of these technologies requires new materials that reduces the content of precious metal without affecting the device efficiency.

I will discuss the challenges opened by these systems to electronic-structure simulations and will present a case study in the context of fuel-cell electrodes, i.e. novel non-conventional CeO<sub>2</sub>-based catalyst with ultra-low metal loading.

We combine DFT simulations with ab-initio molecular dynamics, atomistic thermodynamics, metadynamics, and other enhanced-sampling methods to reveal the new surface chemistry opened by these systems. The calculations are used to characterise the chemical bonding and the reactivity at the electrode active sites in a wide range of compositions and environments, ranging from model surfaces at T=0K in vacuum conditions to realistic wet electrodes at finite temperatures, i.e. chemical reactions at complex solid-liquid interfaces comprising nano-structured surfaces in contact with a solution.

The calculated results allow for rationalising the available experimental data and identify correlations among the reaction mechanisms, thermodynamic efficiency, and local structure of the active sites, thus shedding light on the origins of the amplified reactivity and stability of these novel electrodes.

#### #561 - ADVANCED METAL OXIDE SEMICONDUCTORS FOR SO<sub>2</sub> SENSING

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Atmospheric pollution is still a topical problem in most European cities. Indeed, a significant proportion of population lives in urban areas where the pollutant concentrations often exceed the fixed limits. Air pollution reduces human life expectancy by more than eight months on average and by more than two years in the most polluted cities and regions.

Nowadays, monitoring is usually performed in few fixed stations in urban areas, and with mobile stations (where the conventional equipment is installed on vehicles) for temporary measurement campaigns or occasional environmental impact estimations. The equipment used in these stations is often complex, expensive and difficult to deploy, requiring controlled environmental conditions and frequent maintenance and calibration.

In this frame, the technology of thick film gas sensors is an optimal candidate to be implemented in portable devices having low requirements in terms of power, consumables, maintenance and installation costs. Besides an evident cost-reduction, this implementation will enable on-board correlation and processing of the acquired data, which can be autonomously distributed in a user-friendly format via the integrated wireless network interfaces and/or radio-modems.

Sulfur dioxide (SO<sub>2</sub>) is one of the main atmospheric gaseous pollutants. Their reactivity with the other substances in the atmosphere causes a wide variety of health and environmental negative effects as respiratory disease, visibility impairments, acid precipitants etc.

In this work, SO<sub>2</sub> detection has been carried out through thick film gas sensors based on different functional materials: single oxides as SnO<sub>2</sub>, WO<sub>3</sub> and ZnO synthesized in different morphologies (nano-particles, nano-needles and flower-like microstructures) and mixed oxides as (Ti<sub>x</sub>Sn<sub>1-x</sub>)O<sub>2</sub> and (W<sub>0.9</sub>Sn<sub>0.1</sub>)O<sub>3-x</sub>.

Among them, the best results were offered by (W<sub>0.9</sub>Sn<sub>0.1</sub>)O<sub>3-x</sub> and ZnO nano-particles. In particular, (W<sub>0.9</sub>Sn<sub>0.1</sub>)O<sub>3-x</sub> is the material which exhibited the highest response to SO<sub>2</sub> at the operating temperature of 200 °C.

However, the responses didn't show the bell-shaped behavior or responses increasing or decreasing with temperature. Whereas, a complex behavior as a function of the working temperature and time-dependent it has been found for all sensors. In agreement with Shimizu *et al.*, it has been resulted that SO<sub>2</sub> behaves as a reducing gas at a temperature higher than 400 °C but as an oxidizing gas at a temperature lower than 400 °C.

#### #562 - Coalescence process of SiO<sub>2</sub> supported colloidal Au nanoparticles: experimental analyses and quantitative evaluations

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The controlled growth of nanoparticles (NPs) on surfaces is a powerful tool to create nanostructured materials with desired properties for several technological applications [1]. In particular, metal NPs have attracted much interest due to their potential application in many areas, such as catalysis, sensing, data storage, optoelectronics, biological related areas, plasmonics and photovoltaics [2]. The key step towards reliable solid-state technological applications of metal NPs-based systems is the development of simple, versatile, low-cost, high-throughput methods for the fabrication and manipulation of metal NPs on surfaces. Key requirement, to this aim, is the quantitative understanding of the physical mechanisms governing the NPs growth dynamics under various conditions.

So, we present an experimental investigation on the growth dynamics, induced by thermal processes, of colloidal Au NPs on SiO<sub>2</sub>. In particular, we deposited size-mono-dispersed Au colloidal NPs on SiO<sub>2</sub> surface and performed annealing processes in the 573-1173 K temperature range and 900-3600 s time range. The evolution of the mean NPs size was quantified, by scanning electron microscopy (SEM) analyses, as a function of the annealing time for each annealing temperature. The analyses of the SEM images

suggested us a coalescence process as the main NPs growth mechanism. So, we studied the experimental temporal evolution of the NPs size using the typical relations prescribed by the standard particles coalescence theoretical framework [3, 4]. Fits of the experimental data by such theoretical relations allowed us to determine, in particular, a size-dependent activation energy for the coalescence process of the SiO<sub>2</sub>-supported Au NPs: when the starting diameter of the coalescing NPs increases from 27.5 nm to 53.2 nm, the coalescence activation energy increases from 0.21 eV to 0.34 eV and at higher starting diameters it tends to saturate at about 0.36 eV. The size-dependence of the activation energy is discussed on the basis of the size-dependent cohesive energy of the atoms in the NPs. Finally, the 0.36 eV value is shown to be consistent with a coalescence process driven by surface self-diffusion of Au atoms.

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### #563 - DFT modeling of water oxidation: from molecular catalysts to oxide surfaces

Simone Piccinin - CNR-IOM

Splitting water to produce molecular hydrogen is a promising way to convert and store solar energy in the form of chemical fuels [1]. Efficient catalysts are needed to promote this electrochemical reaction, which, especially on the oxidation side, is extremely challenging, requiring the loss of four electrons and four protons and the creation of the O–O bond. For this semi-reaction several catalysts have been proposed in the past three decades, both heterogeneous (metal oxide surfaces) and homogeneous (transition metals with organic ligands), while Pt is typically used at the cathode. In this talk I will present the results of our theoretical investigations on three systems: (i) an amorphous Co–phosphate material obtained through electrodeposition [2,3]; (ii) hematite surfaces [4,5]; (iii) an inorganic Ru–based polyoxometalate molecular catalyst [6,7]. We show how state-of-the-art theoretical methods help to shed light on the complex mechanism of this reaction. We identify simple descriptors of the catalytic activity, enabling us to rationalize and compare the performance of different classes of catalysts.

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### #564 - Neutron Radiation Damage Testing of Organic Solar Cells

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Polymer-based solar cells have recently emerged as a promising class of photovoltaic diodes, with efficiencies approaching 12%<sup>1</sup>. Since this class of materials allow fabrication of cheap, lightweight and flexible devices, they might be integrated effectively in spacecrafts and thus reduce the associated launching costs. For all these reasons, a detailed study on the effect of radiation exposure needs to be carried out to investigate whether or not these devices are adequately radiation tolerant. Neutron irradiation is a well-established technique to simulate exposure to cosmic rays.

Here we report, for the first time, a study of fast neutron (>10 MeV) radiation tolerance of polymer-fullerene solar cells incorporating either poly(3-hexylthiophene) [P3HT] or poly(2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-b]thiophene) [PBTTT] as electron-donors, and [6,6]-Phenyl C<sub>71</sub> butyric acid methyl ester (PCBM) as the electron-acceptor. We irradiated the devices at three different total-dose of neutrons (1.5, 3 and 4.5 x 10<sup>9</sup> n / cm<sup>2</sup>), observing a general lowering of the efficiencies (40% and 11% for P3HT and PBTTT) already at the lower dose and a higher parameters variability from device to device upon irradiation. Interestingly, PBTTT displays a higher radiation tolerance than P3HT, likely due to its superior structural and conformational stability.

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**#565 - Number and Molecular Brightness and Phasor FLIM methods for mapping p53 tetramers and Metabolic Alterations upon DNA damage**

Michelle Digman (I) - University of California Irvine

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For biological reaction-diffusion systems, live single cell spatiotemporal analysis of protein dynamics provides a mean to observe stochastic biochemical signaling which may lead to better understanding of cancer cell invasion, stem cell differentiation and other fundamental biological processes. Here we describe methodologies used to investigate p53 activity and alteration of the metabolic pathway upon DNA damage. We used the Number and Molecular Brightness (N&B) method to map aggregation processes in the entire cell upon DNA damage with cisplatin (a chemotherapy agent); thus revealing the spatial distribution of events, the site of tetramer formation and the time sequence of the aggregation events with quantitative information about the distribution and size of any intermediate aggregates that are formed. The molecular number and brightness method is based on calculating the average intensity as each pixel of an image and the variance of the fluctuations contributed by those intensities. p53 is a tumor suppressor protein that regulates target genes involved in DNA damage migration and repair. If cells become stressed due to DNA damage, p53 will form tetramers in specific chromatin sites and active genes that trigger cell cycle arrest and/or apoptosis. To gain information regarding fast dynamic processes we use laser beam line scanning on a convention confocal microscope to reveal the transient binding dynamics across the nucleus. Given that p53 has a dual role in promoting oxidative phosphorylation (oxsphos) and glycolysis upon cellular stress and may play an important role in normal growth, development, and tumor suppression, we investigated the effect of metabolic changes upon DNA damage under the same treatment and tested if the concentration of p53 influences the balance between apoptosis and DNA repair. We used the fluorescent lifetime imaging microscopy (FLIM) phasor approach to detect changes in oxsphos and glycolysis. The FLIM/Phasor data show that low concentrations of p53 is enough to trigger glycolytic response in the nucleus of the cells upon DNA damage with cisplatin and under high expression levels, a new lifetime phasor is detected. This new lifetime correlates with dead phenotype cells and may be a new "apoptotic" lifetime signal. Overall, our findings demonstrate that by multiplexing these techniques we have the ability to spatially and temporally quantify p53 activation and map p53's influence in the metabolic pathway. This work is supported in part by NIH grants P50 GM076516 and P41 GM103540.

**#566 - Biophysics of Intrinsic Disorder**

Vladimir N. Uversky (I) - University of South Florida

Intrinsically disordered proteins (IDPs) lack stable tertiary and/or secondary structure under physiological conditions *in vitro*, often resembling 'protein clouds'. Computational studies revealed that IDPs are highly abundant in nature, as ~25-30% of eukaryotic proteins are mostly disordered, and >50% of eukaryotic proteins and > 70% of signaling proteins have long disordered regions. The functional repertoire of IDPs is complementary to that of ordered proteins, with IDPs being commonly involved in regulation, signaling and control pathways, where binding to multiple partners and high-specificity/low-affinity interactions play a crucial role. It is suggested that functions of IDPs may arise from the specific disorder form, from inter-conversion of disordered forms, or from transitions between disordered and ordered conformations. The choice between these conformations is determined by the peculiarities of the protein environment, and many IDPs possess an exceptional ability to be highly responsive to change in their environment and to fold in a template-dependent manner. All this requires a close attention to the odd biophysics of IDPs. In this talk, some key biophysical features of IDPs will be covered. In addition to the peculiar sequence characteristics these unusual biophysical features include sequential, structural, and spatiotemporal heterogeneity of IDPs; their rough and relatively flat energy landscapes; their ability to undergo both induced folding and induced unfolding; the ability to interact specifically with structurally unrelated partners; the ability to gain different structures at binding to different partners; and the ability to keep essential amount of disorder even in the bound form. IDPs are also characterized by the "turned-out" response to the changes in their environment. It is proposed that the heterogeneous spatiotemporal structure of IDPs/IDPRs can be described as a set of foldons, inducible foldons, semi-foldons and non-foldons. They may lose their function when folded, and activation of some IDPs is associated with the awaking of the dormant disorder.

**#567 - Investigation on structural features and antiaggregation properties of chaperonins and chaperone-like protein molecules**

Silvia Vilasi - BIOPHYSICS INSTITUTE, NATIONAL RESEARCH COUNCIL

Molecular chaperones play central roles in many cellular processes, including protein folding, targeting, transport. They are essential in fighting the consequences of protein misfolding and aggregation or enhancing the disaggregation of toxic aggregates by clearance mechanisms. Recent studies have attributed to some chaperones the ability to directly interact with aggregation-prone species of proteins involved in severe neurodegenerative diseases (Alzheimer's disease, Parkinson's disease) and/or to suppress their toxicity. Among these are the principal heat-shock proteins (HSPs), the small HSPs characterized by the alpha-crystallin

domain, but also molecules that exhibit marked chaperone-like activity, like milk caseins or BRICHOS domains. Chaperones exert their protective action by several mechanisms, many of which involve protein disordered regions (IDRs). However, in many cases, the scarcity of structural data has impeded a deep understanding of the recognition and antiaggregation mechanisms. This is crucially important when considering how to screen for and characterize potential inhibitors of amyloidosis. Here we show how two chaperonins, Hsp60 and GroEL, and intrinsically disordered colloids with chaperone-like functions, the milk caseins, can specifically influence fibrillogenesis of A $\beta$ 1-40 amyloid peptide involved in Alzheimer Disease. Inhibition mechanisms are correlated with chaperone structural, self organization and stability properties performed by a battery of biophysical methods and aimed to understand what are molecular determinants responsible for their inhibitory action.

#### #568 - Unfolding of misfolded proteins stimulated by chaperones

Alberto Sassi - *École polytechnique fédérale de Lausanne*

Other Authors: Alessandro Barducci and Paolo De Los Rios ; *École polytechnique fédérale de Lausanne*

Chaperone Hsp70 is a very abundant protein involved in many mechanisms related to protein homeostasis: it assists the proper folding of other polypeptides both during and after translation, it rescues misfolded proteins from aggregates, it enhances protein translocation across membranes and in some cases it takes part in protein degradation. A key feature for these tasks is the fine tuning of the binding affinity between the chaperone and its substrate, performed via ATP-driven conformational changes. When Hsp70 is bound with ADP it has slow rates of binding and unbinding but a high affinity for the substrate, whereas the ATP state is characterized by a faster kinetics but also by a lower affinity. The switch between the two states is obtained mainly via ATP hydrolysis, therefore there is a net energy consumption and the system is driven out of equilibrium. We focus on the role played by Hsp70 in stimulating the unfolding of misfolded proteins. When a protein is kinetically trapped in a non functional metastable state it cannot reach its native state spontaneously in accessible time scales. Interaction with Hsp70 leads to a decrease in the free energy barrier between the native and the misfolded states. The chaperone does not participate actively in the refolding process: it normally enhances the unfolding, leaving to the unfolded protein a chance to spontaneously refold in the native functional state. We implement a kinetic model for a description of this mechanism and illustrate how the necessity of the non equilibrium regime naturally follows from thermodynamic constraints.

#### #569 - An integrated approach to investigate the collective dynamics of the phospholipid bilayer

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The collective dynamics of 1,2-dimyristoyl-sn-glycero-3-phosphatidylcholine (DMPC) bilayers has been investigated by Brillouin neutron scattering and far-infrared (far-IR) spectroscopy. We propose a comprehensive picture of the vibrational features of phospholipid membranes at THz frequencies on the basis of the identified inelastic excitations. The dispersion curves measured by neutron scattering are composed of three branches. The low- and intermediate-energy excitations are interpreted as acoustic transverse and acoustic longitudinal modes, as also suggested by MD simulation results. The high energy branch is described as the superposition of several optic modes of the bilayer lipid chain, on the basis of the consistent scenario provided by the composite far-IR spectra. A strong similarity between the THz vibrational dynamics of lipid membranes and those of water is found.

#### #570 - Investigation on conformational changes in glucose oxidase before and after sol-gel immobilization by means of optical techniques

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Immobilization procedures represent a fundamental stage for technological applications of enzymes. Sol-gel technique is generally considered as a valuable approach to obtain catalytic supports with high chemical stability, superior optical transparency and porosity properties enabling the entrapment of proteins or enzymes. In the present work, structural and dynamic properties of glucose oxidase (GOD) prior and after sol-gel immobilization process have been investigated by using different optical techniques. In particular, we have investigated the optical absorption in the UV-VIS range and the steady-state fluorescence in the FAD region. Moreover we have used time-resolved FAD fluorescence for further studying the changes occurring in GOD dynamic properties

when it is immobilised in a sol-gel matrix. GOD secondary structure has been studied by means of micro-attenuated total reflection (ATR) FT-IR spectroscopy together with deconvolution procedure. Infrared spectroscopy measurements has confirmed that enzymatic activity is preserved and a predominant  $\beta$ -sheet subcomponent is retained by immobilized glucose oxidase. Time-resolved FAD fluorescence has shown that a three-exponential decaying behaviour is observed for both free and immobilized enzymes with three different lifetimes, each of them being characteristic of a distinctive conformational state of the FAD structure. The comparison between lifetime values for free and immobilized glucose oxidase has not shown considerable differences, while the fractional steady-state intensities of the single exponential components have been changed by immobilization procedure an increasing role of the closed and intermediate configuration of FAD moiety. All results reported and discussed in this paper have confirmed once again the efficacy of the sol-gel immobilization procedure for enzymes and proteins with particular attention to the ability of sol-gel technique to well preserve enzymatic activity. In addition, the joint use of different optical spectroscopic techniques has shown to be a very valuable tool for getting a better insight into structural and dynamic properties of immobilized enzymes.

#### #571 - CAT (Confocal-AFM-TIRF) Microscopy : a Novel tool for 3D Investigation of Cells

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CAT (Confocal-AFM-TIRF) microscopy [1] is a combination of an advanced scanning probe microscope (Bioscope Catalyst, Bruker Inc. USA), a confocal microscope (LSM 700, Zeiss GERMANY), and a total internal reflection fluorescence microscope (Laser TIRF 3, Zeiss GERMANY). Devices are mounted on an inverted microscope. AFM allows elasticity and topographical single cell membrane characterization, confocal microscopy permits volume cell investigation whereas TIRF gives information about cell-substrate interface. Their combined use provides a topographic and spectroscopic imaging, and nano-scale adhesion forces and elastic forces mapping of the sample. Therefore the simultaneous combination of all three microscopies gives rise to a complete three-dimensional point of view. By using CAT microscopy we have explored morphological and cytomolecular modifications of cancer cells. In particular we have investigated the effects of ROC-inhibitor (Y-27632) on three different cancer cell lines (MCF-7, MDA-361, SKOV-3) by nanoindentation [2]. ROC inhibitor induced re-arrangement of the actin fibers into the cytoskeleton as visualized by confocal images [1,2]. As further proof of concept, by CAT microscopy we have also investigated the internalization of dendrimers into mitochondrial structures and their targeted colocalization inside cellular compartments [3]. These experiments demonstrate that CAT microscopy is a novel powerful tool for 3D cells investigation.

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**#572 - Fluctuation theorems in classical systems in contact with several baths.**

*Alberto Imparato (I) - Aarhus University*

I will first consider a harmonic chain coupled to two or more heat baths at different temperatures.

I will use this model to introduce and discuss the fluctuation theorem that sets precise constraints on the fluctuations of the heat transfer between the different reservoirs.

I will generalize these results to the case of systems with general interaction potential.

I will then show some experimental results for a system formally equivalent to a harmonic chain with different heat baths, and show that a conservation law for the total entropy exists.

Finally, I will discuss the general case of a system in contact with multiple energy and particle baths, and show that there exists a fluctuation theorem that involves only the energy and the particle currents and that holds at any time.

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**#573 - Spinodals with disorder: from Avalanches in Random Magnets to Facilitated Glassy Dynamics**

*Giulio Biroli (I) - Institute of Theoretical Physics CEA Saclay*

Spinodal phase transitions in presence of quenched disorder play a key role for several out of equilibrium phenomena such as hysteresis in random magnets, glassy dynamics and collective behaviors in social science. In this talk we focus on the quasi-statically driven zero temperature random-field Ising model, which is generically used to model these kind of transitions, and present a complete theory of its spinodal.

We find that the transition is triggered by very rare events: avalanches starting from droplets of the opposite phase that become unstable by a depinning transition.

Our results hold in any finite spatial dimension, thus showing that there is no upper critical dimension contrary to what currently conjectured in the literature. We conclude by discussing the consequence of our results on the current understanding of glassy dynamics.

**#574 - Short-time universality and aging after a quench in isolated quantum systems**

*Andrea Gambassi (I) - SISSA - International School for Advanced Studies*

Recent experimental progresses in the physics of ultracold atomic gases have revived the interest in the dynamics of thermally isolated quantum statistical systems after a sudden change (quench) of their control parameters.

Within a renormalization-group approach and via exact solutions we demonstrate that a system with vector order parameter deeply quenched close to a dynamical critical point exhibits a transient short-time scaling regime which is however dynamically unstable. Within this unusual nonthermal regime, dynamical correlations are characterized by short-time universal exponents and aging, which we investigate both analytically and numerically.



**#575 - Coarsening in inhomogeneous systems***Federico Corberi - Universita' di Salerno**Other Authors: Eugenio Lippiello Dipartimento di Scienze Ambientali, Seconda Universita' di Napoli, Via Vivaldi, Caserta, Italy Marco Zannetti Dipartimento di Fisica "E. R. Caianiello", Universita' di Salerno, via Giovanni Paolo II 132, 84084 Fisciano (SA), Italy.*

We consider the coarsening phenomena occurring in systems where quenched features - such as random field, varying coupling constants or lattice vacancies - spoil homogeneity. We discuss the current understanding of the problem in ferromagnetic systems with a non-conserved scalar order parameter by focusing primarily on the form of the growth-law of the ordered domains, on the scaling properties and on the crossover patterns.

**#576 - Non-Equilibrium Quantum Criticality in One Dimensional Driven-Dissipative Condensates from Engineered Diffusion***Jamir Marino - Technical University of Dresden**Other Authors: Sebastian Diehl (Technical University of Dresden)*

We characterize a novel quantum non-equilibrium universality class, occurring in a driven- dissipative condensate in the presence of one/two body losses and one body pump as well as quartic interactions, in a regime where a engineered strong diffusion term allows for condensation out-of- equilibrium in one dimension, in an analog of a zero temperature condition.

Employing Functional Renormalization Group suited for the non-equilibrium Keldysh action, we provide estimates for the boundaries of the momentum window, where the engineered diffusion dominates over Markovian noise, and a novel quantum critical scaling behaviour out-of-equilibrium can be observed.

In particular, we compute the critical exponent and anomalous dimensions of the Wilson-Fisher fixed point corresponding to this new universality class, and we remarkably find that at this fixed point quantum coherent effects survives to the environmental decoherence, and coexist with dissipative effects. We also comment on the absence of mapping between this novel non-equilibrium quantum critical behaviour in one dimension and its classical counterpart in three dimensions, contrary to what usually occurs for equilibrium phase transitions.

Finally, we briefly discuss a quantum optics implementation of the diffusion term necessary to realise this novel critical regime. Specifically, we show that a spontaneously decaying qubit weakly coupled to the antisymmetric superposition of the microwave bosonic excitations on neighbouring cavities induces additional single particle strong diffusion which favours the new critical quantum regime.

**#577 - Response theory for nonequilibrium stochastic systems***Marco Baiesi - Università di Padova & INFN**Other Authors: Gianmaria Falasco (University of Leipzig), Christian Maes (K.U. Leuven), Urna Basu (K.U. Leuven), Cem Yolcu (Università di Padova), Attilio Stella (Università di Padova), Carlo Vanderzande (Hasselt University)*

Various forms of response (e.g. specific heat, thermal expansion, compressibility, conductivity) for an equilibrium system are all entirely characterized by entropic changes caused by the perturbation, and are related to spontaneous fluctuations of the system via the fluctuation-dissipation theorem. We discuss how this picture is broken out of equilibrium, for systems evolving with a stochastic dynamics. It turns out that the entropy production is not enough for characterizing the linear response far from equilibrium. One also needs to understand how the system's internal activity is modified by the perturbation. This finding is illustrated both for the response to external forces and for the reaction to a change in one temperature when many heat baths keep the system out of equilibrium. We also discuss how somewhat counterintuitive effects as negative differential mobility may be understood with this approach.

**#578 - Dissipative quantum dynamics of multi-level bistable systems***Luca Magazzù - Università di Palermo - Dipartimento di Fisica e Chimica**Other Authors: Davide Valenti (Università di Palermo, Dipartimento di Fisica e Chimica), Angelo Carollo (Università di Palermo, Dipartimento di Fisica e Chimica), Bernardo Spagnolo (Università di Palermo, Dipartimento di Fisica e Chimica)*

We study the dissipative multi-level dynamics of a quantum particle interacting with a bosonic heat bath and confined in a double well potential.

Various physical systems, such as superconducting devices, single-molecule magnets, and chemical reactions, can be described by the model considered.

The time evolution of the system in the spatially localized "discrete variable" representation is obtained by using the Feynman-Vernon path integral approach. This approach is inherently non-perturbative in the system-bath coupling and is thus suited for the strong coupling regime.

The resulting non-Markovian dynamics is given in terms of a generalized master equation, i.e. a set of coupled integro-differential equations for the populations in the discrete variable representation. The kernels of the generalized master equation are derived within different approximation schemes, depending on the coupling regime and bath temperature. By the combined use of Bloch-Redfield and path integral techniques, we establish a phase diagram which accounts for the dynamics of the so-called *double-doublet system*, in various dissipation regimes.

Under appropriate conditions, a master equation with constant rates can be derived from the generalized master equation, allowing for the treatment of both the static and driven case at strong dissipation. Using this master equation a nonmonotonic behavior is found in the escape time from the metastable state of a biased potential.

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#### #579 - Signatures of directed percolation in Rydberg atomic systems

Matteo Marcuzzi - University of Nottingham

Other Authors: Emanuele Levi (University of Nottingham), Weibin Li (University of Nottingham), Juan P. Garrahan (University of Nottingham), Beatriz Olmos (University of Nottingham), Igor Lesanovsky (University of Nottingham)

Directed percolation lies among the simplest instances of genuine non-equilibrium phase transitions. However, until a rather recent study on nematic liquid crystals in two dimensions, no clear evidence of the corresponding universality had been highlighted in real systems. We show that signatures of directed percolation can be highlighted in a strongly interacting ensemble of Rydberg atoms subject to intense dephasing noise. Thanks to the high degree of tunability offered by cold atomic techniques, this approach might allow for the experimental probing of directed percolation in all physical dimensions.

**#580 - Information filtering networks***Tomaso Aste (I) - UCL Computer Science**Other Authors: T Di Matteo (King's College London), G P Massara (UCL London)*

We are witnessing interesting times rich of information, readily available for us all. Using, understanding and filtering such information has become a major activity across science, industry and society at large.

I will show how networks built from dependency measures, both linear and non-linear, can be used to process information while it is generated reducing complexity and dimensionality while keeping the integrity of the dataset. I'll describe algorithms to build these networks and I'll discuss bounds on information retrieval. Applications to financial systems will demonstrate how reliable and useful models can be constructed making use of these information filtering networks.

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**#581 - Kinetics of social contagion***Janos Kertesz (I) - Central European University**Other Authors: Zhongyuan Ruan, Central European University, Hungary; Gerardo Iniguez, Consejo Nacional de Ciencia y Tecnologia, Mexico; Maron Karsai, Ecole Normale de Superieure de Lyon, France*

Diffusion of information, behavioural patterns or innovation follows diverse patterns depending on a number of conditions, including the structure of the underlying social network, the sensitivity to peer pressure and the influence of media. So far, models of complex social contagion have focused on distinguishing between cases where global cascades form from cases without macroscopic spreading. Threshold models have been successful in identifying the conditions for global spreading, leading to phase diagrams in the space of contagion parameters. Yet, little is known about the temporal behaviour of such processes and its governing factors. Here we study analytically and by simulations a general model that incorporates the threshold mechanism capturing sensitivity to peer pressure, the effect of 'immune' nodes who never adopt, and a perpetual flow of external information. While any constant, non-zero rate of dynamically-introduced innovators leads to global spreading, the kinetics by which the asymptotic state is approached show rich behaviour. In particular we find that, as a function of the density of immune nodes, there is a transition from fast to slow spreading governed by entirely different mechanisms. This transition happens below the percolation threshold of fragmentation of the network, and has its origin in the competition between cascading behaviour induced by innovators and blocking of adoption due to immune nodes. We compare the picture suggested by the model with empirical data.

**#582 - Bank-firm credit network in Japan. An analysis of a bipartite network***Luca Marotta - University of Palermo*

We present an analysis of the credit market of Japan from 1980 to 2011, based on a unique dataset reporting credit relationships between banks and publicly quoted firms. The study is performed on the bipartite network of banks and firms where a link between a bank and a firm exists when a credit relationship is present in a given year. By means of the Bipartite Recursively Induced Modules (BRIM) community detection algorithm proposed by Barber, we obtain mixed communities containing both banks and firms. We then introduce a method to track the time evolution of these communities on a statistical basis which takes into account the heterogeneity of the sizes of the different communities. Finally, we investigate the over-expression of attributes of the firms and banks present in each community year by year, using metadata about the type of bank, the geographical location and the economic sector of firms. Altogether, our empirical observations show that the credit market in Japan is a networked market where the type of bank and firm's geographical location and economic sector play a role in shaping the credit relationship.

**#583 - Structure and evolution of the Finnish Parliament through a network analysis of law and budget initiatives***Elena Puccio - Università di Palermo**Other Authors: Michele Tumminello (Dipartimento di Scienze Economiche, Aziendali e Statistiche, Università di Palermo, Viale delle Scienze, 90128 Palermo, Italy), Jyrki Piilo (Department of Physics and Astronomy, University of Turku, FI-20014 Turun yliopisto, Finland), Antti Pajala (Department of Political Science and Contemporary History, University of Turku, FI-20014 Turun yliopisto, Finland)*

We present a study of the network of relationships among members of the Finnish parliament, based on a quantitative analysis of initiative co-signatures, and of its evolution over 15 years.

Our database consists of parliament initiatives, submitted between 1999 and 2014 along with the following information: who submitted each initiative (the proponent), the year it was submitted, its type (budget or law), and all the signers.

We look at the system of initiatives and signers as a bipartite network. In such systems, elements of a given type (initiatives) can only be linked to elements of the other type (members).

To understand the parliament's structure, we constructed a statistically validated network of its members [1], based on the similarity between the patterns of initiatives they signed, and looked for communities in the network. Initiatives are classified in two groups: budget and law. We show that such a subdivision has a remarkable implication on the community structure, indeed, how members interact with each other fundamentally depends on the initiative's type, in such a way that networks ensuing from these two groups show a different clustering.

To gain insight on the nested structure of communities, we constructed a hierarchical tree of members, according to a measure of similarity, based on the number of co-signatures on initiatives [2].

All communities were characterized by members' attributes (gender, party, district, area, coalition and political position) [3]. We followed the changes in communities and their characterization over four different parliaments.

At the local level, we investigated the role played by single individuals, particularly whether they act as leaders or followers, proponents, global or group signers or receivers. To do so we used a measure of reciprocity, that takes into account the number of signatures from a specific member to another and vice versa, and a set of disparity measures aimed at evaluating the in-degree/out-degree imbalance of members.

Finally, we investigated the dynamics of the similarity structure of the system, over the years, with a particular attention to changes in the Parliament composition [4].

Our results provide a quantitative background to current theories in political science. From a methodological point of view, our network approach has proven able to single out both local and global features of a complex social system, such as the Finnish parliament.

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#### #584 - Reaction-diffusion system on complex Cartesian product networks

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From chemistry to biology, passing through physics, spatially extended motifs are found which spontaneously emerge from an ensemble made of interacting microscopic actors. The proto-typical approach to patterns formation in reaction-diffusion processes dates back to Alan Turing's paper on morphogenesis. Here we aim at generalizing the theory of Turing instability for reaction diffusion systems defined on Cartesian networks. These latter are assembled as the Cartesian product of simpler networks, the fundamental building blocks in the process of hierarchical aggregation. To this end we operate in the linear regime and expand the time dependent perturbation on a basis formed by the tensor product of the eigenvectors of the discrete Laplacian operators, associated to each of the individual networks that build the Cartesian product. The dispersion relation which controls the onset of the instability depends on a set of discrete wavelenghts, the eigenvalues of the aforementioned Laplacians. Patterns can develop on the Cartesian network, if they are supported on at least one of its constitutive sub-graphs. Numerical simulations carried out for the Mimura-Murray reaction kinetics confirm the adequacy of the proposed theory.

#### #585 - The development pathways of nations: the heterogeneous dynamics of economic complexity

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In 1960 there were 17 countries with a GDP per capita less than 100 USD and the poorest-richest income ratio among these 17 countries was approximately 2. In 2010 this ratio among the same 17 countries was 100: 50 times larger. How can so similar initial income conditions lead to so different and heterogeneous results? How is it possible to explain the great divergence of developed countries in the last two centuries? What makes a poor country become rich?

Recent results of a new branch - Economic Complexity - set basis for a framework to interpret and explain the extreme heterogeneity of the dynamics of development of nations. The idea behind the concept of *Economic Complexity* is to use the output of a country to determine how fertile the economic system is. In other words, to go from the observable exported products to a

synthetic estimate (fitness) of the level of endowments present in the country, that automatically takes their relationships into account (see Refs. [1-2]).

We will discuss the main results and achievements of Economic Complexity. As an example of them, the metrics for country intangibles allows for quantifying the hidden growth potential of countries by comparing it with money-based figures such as the GDP per capita [3-4]. The analysis of the economic evolution in the plane defined by fitness and GDP per capita pinpoints strongly heterogeneous patterns of evolution and allows to cast economic forecast into the framework of forecasting the evolution of a dynamical system as in the case of weather dynamics. We also observe a strong heterogeneity in the predictability of the economic dynamics. In such a framework, the usual tool used in Economics (i.e. regressions) is no more the appropriate one to deal with such a heterogeneous scenario and new concepts, borrowed from dynamical systems theory, are needed.

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### #586 - A Non-Conventional Metric for the Statistical Characterization of the Air Traffic Management System

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We are presenting an analysis of air traffic data. The aim of this study is to highlight the behaviour of the Air Traffic Controller (ATC) respect to a network optimization operation named direct.

The study is performed on data including all trajectories of flights across Europe, by a comparison between the M1 file and M3 file. The M1 is the last flight plan approved by the Network Manager some hours before departures, and the M3 is the actual radar-tracked trajectory. Especially we focused our attention to the behaviour of ATCs in different countries in a time window of 28 days named Airac.

The trajectories are compounded by a sequence of spatial fixed points (NVP) that typically diverge from the best path route. This infrastructure allows ATCs to direct the air traffic flow on standard air ways, and focuses their attention to a few numbers of special NVPs where the routes converge. As a drawback the not optimal routes force the ATC to modify, where is possible, the routes to enhance the air traffic flow.

As a starting point we observed two mainly stylized facts respect to the ATC operations: the first observation is a significant anti-correlation between ATC operations and traffic, as a second fact we observed that ATCs have an inclination to perform operations as much as the direction of the aircraft diverges respect to the best path routes, in particular this behaviour seems to follow a linear law.

The second part of our work is to define a new local NVP based metric named fork. We show firstly that fork is a good metric to describe direct operations, because it preserves the same stylized fact discussed above, and secondly that it allows us to observe the non-homogeneously spatial distribution of the direct operations.

As third we prove the consistency of this metric by a comparison with a null model based on the hypergeometric distribution, this statistical test permits us to identify a few numbers of special NVPs where the ATC operation can not be explained by a random fluctuation. We therefore analyse the stability of these special points on different Airacs observing a strong complex behaviour that appears when we do not consider the whole system.

This new approach could have an impact in moving from the classical statistical studies to the new network approach based on NVPs [1].

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**#587 - A new method to detect the coupling between time series and its directionality**

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A fast method to detect linear and nonlinear correlations between a pair of time series is proposed. This method, called the Boolean Slope Coherence (BSC), was tested using bivariate time series generated with different models and the corresponding results were compared with those obtained with other well known coupling measures. The comparison shows that the BSC method work well and therefore can be employed to quantify the coupling level between a pair of signals. In addition, with a little modification, the BSC method can be used to establish the coupling directionality. It is shown that the BSC algorithm also works for signals contaminated by noise and was applied to study the coupling level between neurophysiological recordings from visual and motor cortices.

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**#588 - Uncertainties and key open questions in the geological carbon cycle**

*Mike Burton (I) - University of Manchester*

CO<sub>2</sub> emissions from volcanism and metamorphism are key contributors to the geological carbon cycle, and probably contribute at least 3% of the total global CO<sub>2</sub> production, including anthropogenic sources. However, our knowledge of the source term in this cycle, whilst rapidly improving, is still poorly constrained. There remains the possibility that our estimates of the magnitude of the geological CO<sub>2</sub> emissions are significantly underestimated, due to systematic issues with data collection, sparse data, low intensity / large area sources and submarine emissions which are almost completely unquantified. In this context of uncertainty we highlight the fundamental role of the rate of the geological carbon cycle, which will ultimately govern how quickly reductions in anthropogenic emissions produce reductions in atmospheric CO<sub>2</sub> concentrations. Given these large uncertainties in such an important element of the Earth system, with potentially major policy implications, here we attempt to analyse the degree of uncertainty we have on key elements of the geological carbon cycle, and thereby create a probabilistic assessment of the magnitude of CO<sub>2</sub> sources and sinks.

**#589 - Volcanic plumes and particle sedimentation**

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Powerful explosive eruptions are typically associated with sub-vertical or bent-over volcanic plumes that can inject large quantities of gases and particles of various sizes and shapes into the atmosphere, altogether known as tephra. Tephra consists of different components with variable density of both juvenile (fresh magma) and lithic (wall rock) nature and can vary from meter-size blocks and bombs, which are ejected from the vent as ballistics falling within a few kilometres from the source, to micron-size particles, which can be transported by atmospheric winds at continental or global scales. Residence time in the atmosphere mostly depends on particle drag and sedimentation dynamics. Tephra particles may sediment individually, clustered in various types of aggregates or entrapped within sedimentation instabilities and, depending on their sizes, represent different hazards. In particular, impact of ballistic blocks and bombs can significantly damage infrastructure close to the vent; accumulation of lapilli and ash can cause a wide range of damage to communities and ecosystems, while fine ash (<63 µm) can jeopardize civil aviation and the finest micrometric particles can also threaten human health. Depending on the ratio of horizontal wind velocity to plume rise velocity, volcanic plumes can develop as strong (sub-vertical) or weak (bent-over) and eventually reach the Neutral Buoyancy Level (NBL) where their density equals that of the surrounding atmosphere, and start spreading laterally around this level. When the rising plume velocity is significantly larger than the horizontal wind velocity, the plume rises beyond the NBL because of momentum at the top of the plume and, from there, collapses toward the NBL spreading as a gravity current to form an umbrella cloud. Our understanding of both plume dynamics and particle sedimentation is crucial to the characterization of volcanic systems and to an accurate forecasting of the associated hazards and mitigation of risk. Given the complexity of the physical processes, best insights result from a combination of field, experimental, theoretical and numerical studies.

**#590 - Volcanic hazard and instrumental monitoring of volcanic gas emissions**

*Alessandro Aiuppa (I) - University of Palermo*

Mitigating the effects of volcanic eruptions requires quantitative assessment of volcanic hazard, which can be accomplished via modern instrumental volcano monitoring. In the last decades, our ability to monitor, and eventually predict, the activity of hazardous volcanoes has progressed enormously. Despite these advances, however, early warning of eruptions remains challenging, because patterns and consequences of volcanic unrests are difficult to predict. Measuring volcanic gases is key to improved volcano monitoring, because these fluids are thought to be mobile enough to breach to the surface long before magma. Here, we review some of the most recent advances in instrumental monitoring of volcanic gas emissions, putting the accent on recent case study examples in which volcanic gas measurements have fully revealed their utility in eruption forecast.

**#591 - High frequency UV imaging of strombolian explosions**

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We report the first high time resolution measurement (25 Hz) of the SO<sub>2</sub> gas mass emitted during ten discrete explosive events on Stromboli volcano on 25<sup>th</sup> May 2015 using a new dual SO<sub>2</sub> camera system. This unprecedented acquisition frequency revealed a complex explosive outgassing behaviour hardly explainable with a single gas slug bursting at the magma-air interface. Our SO<sub>2</sub> gas flux timeseries show a sequence of multiple bubbles bursting with a time delay in between of a few tenths of a second and each generating a rapid increase of the gas flux. The total masses released during the strombolian explosions ranged from 20 to 50 kg. Our data suggest that strombolian explosions may result from a rapid transition from a degassing regime with separated bubbles

bursting at the surface (passive degassing) to an explosive degassing regime characterized by several interconnected bubbles linking the shallow conduit to a more deep and gas-rich magma.

### **#592 - Quantifying lava flow risk at Mt. Etna: constraints imposed by historic eruptions and numerical simulations**

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Quantifying lava flow risk at Mt. Etna: constraints imposed by historic eruptions and numerical simulations

A. Cappello, A. Michaud-Dubuy, C. Del Negro

With the frequent effusive eruptions of Mount Etna throughout the 20th and early 21st centuries, lava flows have been the most common threat to 900,000 people and property around the volcano. Lava flows have caused significant social and economic damage in the area around Mt. Etna. Major examples include the 1928 eruption, when the town of Mascali was completely destroyed; the 1981, when the town of Randazzo was narrowly missed but huge damage were caused to roads, railways, electricity and telecommunications networks; or in 2001 when tourist facilities close to the summit area were destroyed causing economic loss. Efforts to mitigate risk can only be implemented after the lava flow hazards are characterized. Improving both lava flow hazard and risk assessment is therefore crucial. Following previous studies on lava flow hazard conducted at the INGV (Istituto Nazionale di Geofisica e Vulcanologia) of Catania, we evaluate the inundation risk by lava flow for the Mt. Etna region in Sicily (Southern Italy) using a GIS-based methodology, which involves different stages. First we identify the elements-at-stake by collecting data gathered from national and regional geographic webportals. These data were organized in GIS environment into four groups: population, critical facilities (including hospitals, army, security, governance, buildings of historical value and industrial infrastructures), others buildings and networks (including railways, roads and energy networks), and land use. Using weighted linear combination and pairwise comparison matrices, we converted the distribution of these data in five exposure maps, which were finally combined in the long-term risk map from lava flow inundation at Etna. In order to provide a user-friendly interface and allow an easy access, all maps were included in a module of our web-GIS framework LAV@HAZARD. Our work provides a more complete risk assessment and aims at increasing consciousness about volcanic hazards.

### **#593 - The December 28, 2014 Mt. Etna lava-fountaining event: a deep magma recharge from a multidisciplinary approach**

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During 2011-2014, Mt. Etna produced about 50 episodic short-lasting eruptions of predominantly explosive characteristics with respect to lava output. These episodes were fed by New South-East summit crater (NSEC) and characterized by transition from mild intra-crater explosive activity that eventually evolved in intense strombolian explosions to pass to fire fountaining and lava effusion. All these eruptions were accompanied by very slight ground deformation (observed only by tiltmeters and dilatimeters) and by no rock failure-related seismicity. However, on 28 December 2014, a paroxysmal episode took place showing peculiar geophysical and volcanological features, i.e. intense ground deformations and rock failure-related seismicity were observed, as well as the opening of an eruptive fissure, suggesting the emplacement of a dyke.

In this work, we used integrated geophysical (seismic, tilt, GPS), geochemical, and volcanological observations to investigate into the likely triggering mechanisms on the basis of the peculiarities of the 28 December eruptive episode and to propose an explanation for the occurrence of this anomalous lava fountain in the framework of the episodic paroxysmal phases supplied by Mt. Etna since 2011. The multiparametric approach allowed us to identify a pressurization phase of the plumbing system, leading to the eruptive episode. Such a phase was initially observed by means of GPS data showing an inflation pattern from August 2014, interpreted as resulting from an elongated ellipsoidal pressure source centred at  $-4.5$  km b.s.l. depth beneath the summit crater area of the volcano with an estimated volume variation of  $-2.45 \times 10^6$  m<sup>3</sup>. From mid-October, the pressurization started involving also the shallow plumbing system ( $> 1$  km a.s.l.), as inferred by both the gradual increase of the long period event amplitudes, the progressive migration of the tremor centroids at deeper depth and by increase of the ratio between SO<sub>2</sub> and HCl gas species (that start to exsolve from parental magma at different depth,  $<4$  km and  $<2$  km below the surface, respectively). In addition, the multidisciplinary approach of this study gave insights into the mechanisms of the dyke emplacement that were reconstructed in detail by means of both time-dependent modeling, applied on GPS and tilt ground deformation data, and seismic data.

### **#594 - Multigas spectrometers for the analysis of volcanic emissions**

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We present a set of three analyzers for the in-field measurement of the concentrations of molecular species typical of volcanic emissions: H<sub>2</sub>O, CO<sub>2</sub>, HCl, HF, SO<sub>2</sub>. Moreover the isotopic ratio <sup>37</sup>Cl/<sup>35</sup>Cl is measured in the emitted hydrogen chloride.

These instruments have been developed within the frame of the ERC Project CO2Volc (Grant 279802). The Project aims to the measurement of several molecular species in the volcanic plumes.

The analyzers are based on molecular spectroscopy. For each of them the volcanic plume interacts in a multipass cell with two laser beams at suitable wavelengths. For SO<sub>2</sub> only an UV, fiber coupled LED is used. In the latter case the absorption figure is analyzed by means of a compact spectrometer, while for the other gases concentrations and isotopic ratio are retrieved by fitting the transmission of the scanning lasers across the cell with theoretical curves.

We report here the results of the laboratory checks of the instruments, and the results of measurement campaigns carried out on Etna and Vulcano. The campaigns aimed to verify not only the in-field performances of the analyzers but also to assess their robustness in such a hostile environment.

The absolute values of the concentrations and their correlations will be shown, together with in-field precision and accuracy.

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**#595 - Magnetoencephalography as a tool for the study of brain connectivity***Vittorio Pizzella (I) - University of Chieti-Pescara*

The understanding of the functional mechanisms of the human brain, a highly complex system featuring  $10^{12}$  deeply interconnected neurons, is undoubtedly one of the major challenges of this century. Nowadays, there is a general consensus on the idea that the uniqueness of the human brain heavily relies on how neurons are connected and how these connections modulate over time, rather than on the overall brain size. To the end of non-invasively investigate these aspects, in addition to Magnetic Resonance Imaging (MRI), functional techniques able to catch brain connectivity on a timescale relevant for behavior are being used. Among the different choices, magnetoencephalography (MEG) is the best non-invasive technique to probe brain functional connectivity.

In this talk, the principles of MEG will be briefly reviewed, the technological challenges that must be faced to successfully measure the neuromagnetic field will be discussed, and the main results of the technique in the study of brain functional connectivity will be given. Synchronized neuronal currents induce weak magnetic fields outside the head that can be measured with MEG through highly sensitive detectors. Indeed, low temperature superconducting magnetometers, namely LTC-SQUIDS (Superconducting QUantum Interference Devices), have been used since over 30 years and are still the only detectors used in commercial devices, thanks to their excellent noise figure at ultra-low frequencies. Recently new detectors are being developed: HTC-SQUIDS working at 77K, but also microfabricated atomic magnetometers based on laser spectroscopy of rubidium vapor which have shown potential promising performances. The magnetic field measured with MEG can be used to infer brain activity through solving an inverse problem and, subsequently, to study functional connectivity, e.g. through the estimation of the phase relationship between the activity at two brain sites. Indeed, the study of brain electrical activity with invasive measurements suggests that precise timing of neuronal activity is essential for a successful integration of information in the brain, and magnetoencephalography, with its excellent time resolution, is a perfect tool for tracking the flow of information between neuronal pools.

**#596 - Magnetic Resonance Imaging from kHz to GHz: Hardware Developments and Biomedical Applications***Marcello Alecci (I) - University of L'Aquila*

Despite the fact that Magnetic Resonance Imaging (MRI) is a mature technology, now present in most hospitals, its development has not slowed to any significant extent over the past three decades. This is probably due to the interplay between academic and industrial research, driving the continuing development of new methods and hardware, with ever increasing biomedical applications.

We will, first, review the latest advancements in MRI hardware and, then, discuss a selection of biomedical applications, ranging from ultra-low field (kHz) to ultra-high field (GHz). In particular, we will focus on the radiofrequency detection chain that in the past decade has undergone radical changes thanks to the development of multi-channel transmit/receive MRI systems [1] and travelling wave detection [2].

Special attention will be provided to the biomedical use of multiple-tuned radio frequency sensors suitable for the concurrent detection of proton ( $^1\text{H}$ ) and other X-nuclei nuclear spins ( $^7\text{Li}$ ,  $^{23}\text{Na}$ ,  $^{39}\text{K}$ ,  $^{35}\text{Cl}$ ,  $^{17}\text{O}$ ) [3-4].

Another novel area that will be discussed is the development of multimodality imaging methods, where MRI is being integrated with MEG [5-7] or PET systems [8-9], to take advantage of wider molecular imaging contrast mechanisms and/or ultra-fast acquisition times, both suitable for functional studies in animal models and humans.

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**#597 - Improvements to the Signal-to-Noise Ratio in long Source-Detector Separation with Silicon Photomultipliers, bringing increased potentiality to human brain NIRS applications***Roberto Pagano - CNR-IMM*

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Near-Infrared Spectroscopy (NIRS) is a method of non-invasive optical spectroscopy based on the relative transparency of biological tissue to near-infrared light. Applications cover pharmaceutical and medical diagnostics, sports medicine, research in functional neuroimaging and urology etc.

In neuroscience research, functional near-infrared spectroscopy and imaging (fNIRS/fNIRI) have become widely used technologies over the last 20 years. In the brain the variation of O<sub>2</sub>Hb and HHb concentrations in the blood, due to the neurovascular coupling, is caused by an increase in the oxygen consumption due to cortical activity. fNIRS uses near infrared sources and detectors to measure changes in the absorption due to neurovascular dynamics in response to brain activation.

The use of Silicon Photomultiplier (SiPM), the youngest detector in the family of silicon detectors, in a CW-fNIRS system is potentially able to increase the source-detector-separation (SDS). The penetration sensing depth in human brains would also increase, thanks to its higher responsivity compared to traditional semiconductor detectors and its outstanding Signal-to-Noise-Ratio (SNR), very close to the one of traditional Photomultiplier Tubes (PMT) [1,2].

In this work we studied, using standard electronics equipment, the limits reachable, in terms of SNR as a function of the SDS and of the minimum optical source power required, of a CW-NIRs system based on LED sources having wavelengths in the range of 700-950 nm, and a SiPM detector with a 4mm<sup>2</sup> area developed by STMicroelectronics [3,4].

In particular, we measured the response of a SiPM placed in direct contact with plastic phantoms (produced by the INO Biomimic Optical Phantom division) having four layers: the Skull/Scalp, the Cerebral Spinal Fluid, the Grey and the White Matter layers. They have different thicknesses mimicking a real human head, at different SDS (2-7 cm), source optical powers and LED repetition rates. Results have been compared with Monte Carlo (MC) optical simulations and with a calculated theoretical minimum SNR required to have enough accuracy to detect small variations in the O<sub>2</sub>Hb and HHb concentrations [1]. The measured SNR, for a LED operating at 40 mA and with repetition rates of 2 kHz, is higher than the calculated minimum for a SDS up to 6 cm. At lower frequency even a higher separation can be used. To our knowledge this SDS has never been achieved by a CW-NIR system and could bring new advances in neuroscience research.

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#### #598 - ON-CHIP DEVICES FOR MECHANOBIOLOGY STUDIES AND INVESTIGATION OF CELLULAR FUNCTIONS VIA MAGNETIC PARTICLES AND MICROFLUIDIC CHANNELS

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In vitro tests and analysis are of fundamental importance for investigating biological mechanisms in cells and bio-molecules. The application of controlled forces to activate specific bio-pathways and investigate their effects, mimicking the role of the cellular environment, is becoming a prominent approach in this field [1]. In particular, cellular deformation and migration are deeply studied as their comprehension can path the way for cancer treatment and diagnosis.

In this work, we present two different on-chip devices for mechanobiology studies. The first one is based on the fine manipulation of magnetic particles, exploiting Domain Wall Tweezers technology [2], in which magnetic Domain Walls (DWs) in ferromagnetic conduits are used for trapping and finely manipulating single superparamagnetic beads properly functionalized.

To this scope, nanometric Ni<sub>80</sub>Fe<sub>20</sub> rings are patterned on a chip where cells are afterwards cultured and a pair of DWs, which attract and drag magnetic nanoparticles, are nucleated and displaced through the application of an external magnetic field. In this way, we demonstrate the possibility to handle with high resolution (down to 100 nm) magnetic beads to a target cell and to assess localized forces which are finely tuned in the pN-nN range.

In order to properly investigate the cellular migration of cancerous cells, a second device based on polydimethylsiloxane (PDMS) micrometric channels is fabricated by soft lithography. Cells are injected by micropipetting and their mobility inside channels of different dimensions is studied. The channels have a variable section, in order to highlight mechanisms (e.g. specific gene expression) activated to regulate cellular plasticity when an increasing deformation of cytoplasm or nucleus is required to migrate.

The cellular response and behavior in all the experiment is monitored in real time by means of optical methods, like confocal microscopy.

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#### #599 - Superparamagnetic iron oxide nanoparticles enriched fibrin hydrogels as an antibacterial sealing for implants

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The occurrence of microbial biofilms is rather common in biomedical implants, such as joint prostheses, catheters, mechanical heart valves, pacemakers. Biofilms are matrices of extracellular polymeric substances produced by bacteria, containing one or multiple species of microorganisms (bacteria or yeasts). Such matrices are often responsible for the development of chronic infections. Indeed, they act as barriers to prevent antibiotics to reach bacteria, making biofilms highly resistant to antibiotic therapies<sup>1</sup>. From here, the need of developing new antibacterial strategies.

In this contest, in the last years, some studies suggested the employment of functionalized superparamagnetic iron oxide nanoparticles (SPION) as carriers for targeted drug delivery. Indeed, with respect to other nanoparticles, SPIONS have the advantage that they can be targeted to the infection site, and forced to penetrate the biofilm, by means of the application of a magnetic field<sup>2</sup>. Interestingly, in 2009 Taylor et al. reported that prosthetic biofilm formation would be prevented by the employment of not-functionalized SPION<sup>3</sup>, although the origin of the highlighted antibacterial properties is nowadays matter of debate.

Here we present an experimental study carried out on SPION-rich-fibrin-hydrogels, with the aim of obtain a biocompatible hydrogel with intrinsic antibacterial properties. Fibrin is a physiological blood component, involved in hemostasis, resulting from the enzymatic action of thrombin on the protein fibrinogen. It is a versatile biopolymer, which combines different important properties such as biocompatibility, flexibility, adhesion. For its properties, fibrin is widely used as a scaffold in tissue engineering and as a sealing for implants in medicine and surgery<sup>4</sup>. In this study we produced hydrogels at different ratio of fibrinogen, thrombin and nanoparticles concentrations. The action of an applied magnetic field was investigated after and during the polymerization. Morphology of the hydrogels was investigated by means of scanning electron microscopy (SEM) and atomic force microscopy (AFM) measurements.

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#### #600 - Synthesis and characterization of a new insulin conjugated nanogel for biomedical application

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Insulin, a metabolic hormone involved in glucose metabolism, plays also a neuroprotective role in the central nervous system being able to revert the cytotoxic processes induced by A $\beta$ <sub>42</sub>, a peptide involved in Alzheimer's disease. To reach the brain insulin have to cross the BBB therefore an additional delivery strategy results to be necessary. For these aim we performed an insulin conjugated nanogels (NGs-In). Nanogels (NGs) have a great potential in the development of "smart" nanocarriers for (bio)molecular drugs and contrast agent for bioimaging. They are formed by physically or chemically crosslinked polymer networks, characterized by a large and flexible surface available for multivalent bioconjugations. NGs can be produced with high yields and through-puts by pulsed electron-beam irradiation of dilute aqueous solutions of water-soluble biocompatible polymers. In this work, a carboxyl functionalized nanogel system (NG), generated by pulsed e-beam irradiation of a semi-dilute poly(N-vinyl pyrrolidone) (PVP) aqueous solution in the presence of acrylic acid, with an average diameter in the 60-70 nm range (PDI<0.3) was used as a substrate to generate chemically stable insulin-grafted PVP NGs. In particular, grafting was carried out using human insulin without (PVP-g-insulin) or with fluorescein isothiocyanate labeling (PVP-g-insulin-FITC). The hydrodynamic dimensions of NGs before and after grafting ("naked NGs" and "grafted NGs") were investigated by Dynamic Light Scattering. For the biological application, as first step, we have evaluated the biocompatibility and immunogenicity of NGs, at different concentration, on neuroblastoma LAN5 cells and PBMCs. Moreover we have demonstrated the capacity of NGs to protect the insulin from protease action by a resistance proteinase assay. Finally, the biological effect and neuroprotection of NGs-In has been verified.

#### #601 - Phenol compounds as new materials for Electron Spin Resonance (ESR) dosimetry in clinical photon and electron beams

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In the last decades several research laboratories have shown an increasing interest aimed at extending the applicability of Electron Spin Resonance (ESR) dosimetry to radiotherapy with different types of radiation beams. ESR is a spectroscopic method for investigating the structure and dynamics of such paramagnetic species. Free radicals are known to be produced when a compound is irradiated with ionizing radiations. The concentration of radiation-induced free radicals is proportional to the energy released inside in the medium and this allows for dosimetric measurements through ESR technique which able to quantitatively determine the radical concentration. The use of alanine as a dosimetric material gave the possibility to apply ESR spectroscopy for high-dose standardization and dose control in radiation processing. The ESR dosimetric method has many advantages such as simple and rapid dose evaluation, the readout procedure is non-destructive, linear response of many organic and inorganic compounds. ESR detectors show a behavior that suggest possible applications for various kinds of beams used for radiation therapy. Nowadays, the most widely used organic compound as a dosimeter is the alanine. However, many researches are in progress with the aim at improving sensitivity of ESR dosimetry for doses much smaller than 1 Gy. More sensitive materials than alanine are needed to make the ESR dosimeter competitive with other dosimetry systems.

Our research group has started an investigation of the ESR response of some phenols compounds for possible ESR dosimetric applications suitable features, such as high efficiency of radiation-matter energy transfer and radical stability at room temperature. Phenols are compounds possessing a benzene ring attached to a OH group. After irradiation the final product is a stable phenoxy radical. The stability of such radical can be improved by adding other alkyl chains which can be attached to the benzene ring. In particular, the phenol *octadecyl-3-(3,5-di-tert.butyl-4-hydroxyphenyl)-propionate* gave interesting results. Moreover, its high molecular weight, the low volatility and the compatibility with the dosimeter binding material (wax) are advantages with respect to lower molecular weight phenols.

In this work we report the ESR investigation of phenols exposed to clinical photon and electron beams. The dosimetric features of these ESR dosimeters (dependence on microwave power and modulation amplitude, their response after gamma and electron irradiations, dependence on beam type and energy, the detection limits for both beam typologies, signal stability after irradiation) were investigated and the results are reported.

#### **#602 - Evaluation of the effective resolution of an optical flatbed scanner for radiochromic films analysis**

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In radiation dosimetry there are numerous problems associated with the measurement of isodose curves and depth-dose distributions in high-gradient regions using conventional measuring systems such as ionization chambers, semiconductors and thermoluminescent detectors (TLDs).

These difficulties have been overcome by the introduction of radiation dosimeter with high spatial resolution which does not require a special developmental procedure and gives permanent absolute values of absorbed dose with an acceptable accuracy and precision and ease of handling and data analysis: the radiochromic film. Radiochromic dosimeters color directly, do not require chemical processing and their color change indicates exposure to radiation. Image formation occurs as a polymerization process, in which energy is transferred from ionizing radiation, initiating color formation through chemical changes.

The radiochromic films, after being irradiated, can be scanned with a professional commercial optical flatbed scanner. In this way it is possible to obtain a calibration curve that links the blackening of the film with the absorbed dose. Gafchromic® films are undoubtedly the most widely used in most modern medical centers and they are divided into two main groups: films dedicated to radiotherapy (EBT2 and EBT3) and films dedicated to diagnostics group (the set of XR films). The main difference between them is that the former are analyzed with the flatbed scanner in transmission mode, the seconds in reflection mode. Although the maximum resolution of these films is often associated to the size of the activated monomers in the blackening process, the instrument that plays the main role is the optical scanner that captures an image of the film to associate with the absorbed dose. The resolution of a scanner is expressed in dpi (dot per inches), which expresses the number of dots printed or displayed on a line long one inch and is related to the amount of image information provided by a input device. For this reason, a study investigating the effective spatial resolution of commercial scanners used for radiochromic films has been conducted. For this purpose XR-QA2 films, specifically designed as a Quality Assurance (QA) tool for radiology in a process-less environment have been used. These films have a sensitivity range from 0.1 to 20 cGy, can be handled in room-light and have to be read in reflection mode with an optical scanner. The quantitative evaluation of the resolution of the scanner in reflective mode was performed with the theoretical method of the Modulation Transfer Function (MTF), that is useful in evaluating the performance of any optical device. In this way it was possible to compare the nominal resolution of the optical scanner with that experimentally evaluated, that depend on the combined properties of the light sensor, electronics, optics and mechanical components, and the protocol of image acquisition.



**#603 - Correlations in brain activity***Lucilla de Arcangelis (I) - Second University of Naples*

Neuronal avalanches are a novel mode of spontaneous brain activity, experimentally found *in vitro* and *in vivo*, which exhibits a robust critical behaviour. Avalanche activity can be modelled within the self-organized criticality framework, including threshold firing, refractory period and activity-dependent synaptic plasticity. The size and duration distributions confirm that the system acts in a critical state, whose scaling behaviour is in agreement with experimental data. Interestingly, the critical behaviour is robust with respect to network features but shows interesting features on modular networks.

The temporal organization of neuronal avalanches can be characterized by the distribution of waiting times between successive events. Experimental measurements in the rat cortex *in vitro* exhibit a non-monotonic behavior, not usually found in other natural processes. Numerical simulations provide evidence that this behavior is a consequence of the alternation between states of high and low activity, leading to a dynamic balance between excitation and inhibition. This behavior has been verified on a larger scale, i.e., on fMRI data from resting patients, where activity variations with opposite sign are correlated over a temporal scale of few seconds, suggesting a critical balance between activity excitation and depression in the brain.

**#604 - A novel view of brain function: emergent neural dynamics near criticality***Dante R. Chialvo (I) - Conicet*

A large repertoire of spatiotemporal activity patterns in the brain is the basis for adaptive behaviour. Understanding the mechanism by which the brain's hundred billion neurons and hundred trillion synapses manage to produce such a range of cortical configurations in a flexible manner remains a fundamental problem in neuroscience. One plausible solution is the involvement of universal mechanisms of emergent complex phenomena evident in dynamical systems poised near a critical point of a second-order phase transition. We review recent theoretical and empirical results supporting the notion that the brain is naturally poised near criticality, as well as its implications for better understanding of the brain.

**#605 - Self-organized criticality in cortical ensembles is promoted by concurrent scale-free and small-world networks***Paolo Massobrio (I) - University of Genova*

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The spontaneous activity of cortical networks is characterized by the emergence of different dynamic states. Although several attempts were accomplished to understand the origin of these dynamics, the underlying factors continue to be elusive. In this work, we specifically investigated the interplay between network topology and spontaneous dynamics within the framework of self-organized criticality (SOC). The obtained results support the hypothesis that the emergence of *critical states* occurs in specific complex network topologies. By combining multi-electrode recordings of spontaneous activity of *in vitro* cortical ensembles with theoretical models, we demonstrate that different 'connectivity rules' drive the network towards different dynamic states. In particular, scale-free architectures with different degree of small-worldness account better for the variability observed in experimental data, giving rise to different dynamic states.

Keywords: connectivity, cortical assemblies, neuronal avalanches, self-organized criticality, simulations

**#606 - Looking into the architecture of the brain with MRI: quantification of non-Gaussian water diffusion by Diffusion Kurtosis Imaging (DKI)***Giorgio Collura - Department of Physics and Chemistry, University of Palermo and INFN Catania Section*

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The analysis of diffusion tensor imaging (DTI) allows to evaluate *in vivo* and in a non-invasive way the process of diffusion of water molecules in biological tissues. The peculiar organization of some biological tissues influences this phenomenon making it anisotropic and therefore well evaluable with these techniques. Changes in tissue anisotropy can also be found in many diseases without any signal intensity variation on conventional MR pulse sequences since they are intimately related to intrinsic microstructural changes.

Despite all these important applications, DTI fails to fully utilize the MR diffusion measurements that are inherent to tissue microstructure. DTI implicitly assumes that water molecule diffusion occurs with a Gaussian distribution of diffusion displacement. This assumption has been experimentally demonstrated to be not always suitable in both white matter and gray matter. Moreover,

the simplified description of the diffusion process *in vivo* by a 2nd-order 3D diffusion tensor prevents DTI from being truly effective in characterizing relatively isotropic tissue such as GM. Even in WM, the DTI model can fail if the tissue contains substantial crossing or diverging fibers.

Jensen et al. introduced diffusion kurtosis imaging (DKI), a higher order diffusion model that is a straightforward extension of the DTI model. DKI is an approximation of the logarithmic expansion of the DWI signal decay up to the  $b^2$  term and neglects the  $b^3$  terms. DKI gives a dimensionless measure that quantifies the deviation of the water diffusion displacement profile from the Gaussian distribution of unrestricted diffusion, providing a measure of the degree of diffusion hindrance or restriction.

The aim of this work is the definition of an MRI protocol for Diffusion Kurtosis Imaging (DKI) by using a 1.5T clinical scanner and the development of a software for DKI analysis.

Indeed, the extensive application of DKI in a clinical routine must deal with several difficulties. The most important is the long acquisition time. In clinical applications the real issues is to find a good compromise between acquisition time and robustness of the fit. Another major problem of DKI is that these DWI images are usually acquired with an echo planar imaging (EPI) sequence and also require high b-values, resulting in a low SNR of acquired diffusion weighted images. The MRI protocol that we used for DKI acquisitions at 1.5T clinical scanner is chosen with the aim at achieving the above mentioned compromise.

The images were analyzed with a software developed by our research group and able to reconstruct typical DKI maps. This software provides the values of Kurtosis Tensor, Diffusion Tensor, and parametric maps related. Python language was used to develop this software inspired and realized in collaboration with a team of the "Dipy" software project.

### #607 - Neuronal signalling viewed through newly designed neurobiosensors

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Neuronal signals timely regulate the function of complex neuronal networks that form the human brain. They are generated by molecular events that derive from rapid conformational changes of integral membrane proteins (ion channels, receptors and transporters). Membrane ion channels and receptors thus generate electrical signals (action potentials), regulate neurotransmitter release (synaptic transmission) and control the activity of complex neuronal networks, allowing for instance, the rapid exchange of information between brain and peripheral nervous system.

Monitoring the signals generated by single neurons or neuronal networks *in vitro* and *in vivo* is a central task to understand the molecular basis of the central nervous system physiology and to identify the molecular targets for the treatment of neurodegenerative diseases (Alzheimer, Parkinson, depression, sleep disorders, chronic stress, ...). To date exist a large number of multi-electrode arrays (MEAs) made of different material (TiN, ITO, CMOS, MOSFET, carbon-based, conductive polymers) able to detect the electrical activity of neuronal networks, but exist few examples of *lab-on-chips* capable of detecting the quantal release of neurotransmitters from neurons or neuroendocrine cells with high time resolution and signal-to-noise ratio.

With the idea of developing new planar diamond-based biosensors able of detecting action potentials, synaptic activity and optical signals in neurons and neuroendocrine cells, we have tested a new series of devices made of boron-doped nanocrystalline diamond (NCD-MEAs) (Gosso et al. *J. Physiol.*, 2014; Conte et al. *Phys. Stat. Sol. A*, 2015) and micro-graphitic channels buried on diamond mono-crystals ( $\mu$ G-MEAs) (Picollo et al. *Adv. Mat.*, 2013; Picollo et al., *Sensors*, 2015) of different geometries. The chips, with increasing number of microelectrodes (2x2, 3x3, 4x4, 8x8), are made with sensitive areas of either low- or high-density depending on whether the recordings is from population of cells, excitable tissues, neuronal networks (low-density) or single cells (high-density). In the latter case the chip can resolve the secretory activity of cell micro-domains.

The rationale of using these two classes of MEAs to study "neuronal signals" *in-vitro* and *in-vivo* will be discussed together with the expected future applications of more advanced devices.

### #608 - Heterogeneous mean field approach to neural networks

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We discuss how one can approach the study of neural dynamics in disordered dense uncorrelated networks by a mean-field approach that preserves disorder effects in the thermodynamic limit. The method allows to obtain an effective description of the model at hand by reducing the dynamics of single neurons to the one of classes of neurons characterized by their in-degree connectivity. Moreover, the method allows to solve the global inverse problem of reconstructing the network structure (including the fraction of excitatory and inhibitory neurons) from the properties of the global synaptic activity field.



**#609 - The effects of Alzheimer's disease on hippocampal CA1 pyramidal neurons: an experimental and computational study**

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The effects of Alzheimer's disease (AD) on hippocampal CA1 pyramidal neurons were studied in wild type (*wt*) and transgenic (Tg2576, *tg*) mice, using patch clamp techniques in whole cell configuration as well as with computational models.

Experimentally, the response of neurons was recorded under current clamp conditions, in the presence of GABAergic inhibition blocker; a number of physiological parameters (e.g. number of spikes, latency and adaptation) were analyzed to investigate the differences between *wt* and *tg* cells. The effects on synaptic integration at proximal vs distal synaptic inputs were also evaluated. The results showed that the cells *tg* are more excitable than the *wt* ones; a greater synaptic integration was also observed in *tg* cells.

A computational model for *wt* and *tg* CA1 neurons was also implemented, starting from published models [1,2] optimized to reproduce the number of spikes as a function of the input current obtained experimentally. The model suggests that, under our experimental conditions, the mechanisms most affected by AD are the input resistance and the fast sodium current, and predicts an increase in the neuron's input resistance and a decrease in the sodium current. These changes may be directly related to the early effects of  $\beta$ -amyloid peptide accumulation on the neuronal membrane, where they would act at the same time as an excitatory mechanism (increasing the input resistance by reducing passive losses) and as an inhibitory mechanism (by partially blocking Na channels). The overall dynamical competition between these two effects may explain why the early stages of AD can be coupled with episodes of epileptic seizures.

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**#610 - Superconductivity in Flatland: Universal Enhancement in 2D Semiconductors at Low Doping by Electron-Electron Interaction***Francesco Mauri (I) - CNRS Paris**Other Authors: Matteo Calandra, Paolo Zocante*

The occurrence of superconductivity has been reported in several two-dimensional (2D) semiconductors, such as transition metal dichalcogenides or cloronitrides (ZrNCl, HfNCl). In all these systems, a metallic state can be achieved and controlled by intercalation or by gating in a field-effect transistors. Unexpectedly, in the layer compound  $\text{Li}_x\text{ZrNCl}$ , the superconducting transition temperature ( $T_c$ ) increases by decreasing the doping ( $x$ ), reaching a maximum of 15 K at the metal-insulator transition. ZrNCl is a layered large gap semiconductor, with an extremely weak interlayer coupling and 2 equivalent valleys with isotropic mass tensors in the conduction band. The Li intercalation acts as a rigid filling of the conduction band with  $x$  electrons. The bands are almost parabolic for doping  $x < 2/9$ .  $\text{Li}_x\text{ZrNCl}$  is thus a realization of a 2D 2-valley electron-gas. The presence of multiple valleys is the key ingredient to explain the observed doping-dependence of  $T_c$ . Indeed in a 2-dimensional multivalley semiconductor, at low doping, even a moderate electron-electron interaction enhances the response to any perturbation inducing a valley polarization. If the valley polarization is due to the electron-phonon coupling, the electron-electron interaction results in an enhancement of the superconducting critical temperature. By performing first principles calculations beyond DFT, we prove that this effect accounts for the unconventional doping-dependence of  $T_c$  in  $\text{Li}_x\text{ZrNCl}$ . I will conclude discussing the conditions to maximize  $T_c$  in weakly doped 2-dimensional semiconductors.

Matteo Calandra, Paolo Zocante, Francesco Mauri, Phys. Rev. Lett. 114, 077001 (2015).

**#611 - Formation and processing of silicon-metal interfaces below epitaxial graphene.***Rosanna Larciprete (I) - CNR-ISC*

Silicon intercalation below epitaxial graphene (Gr) has the potential of being the feedthrough towards the fabrication of Gr-Si heterostructures compatible with the current Si-based microelectronic techniques. Chemical manipulation of these systems to achieve direct material synthesis below graphene or stable doping configurations could be the key for the development of Gr-based nanodevices.

It has been proven that the intercalation of Si atoms at Gr/metal interfaces leads to the recovery of the intrinsic electronic behavior of graphene [1]. However the interaction between Si atoms and metal substrate, which might occur through simple adsorption, element intermixing or even silicide phase formation, can strongly alter the chemical and electronic properties of the substrate surface, influencing the charge state of graphene. We have used electronic and structural diagnostics with synchrotron radiation to follow the formation of Gr/Si/Ir(111) and Gr/Si/Ru(0001) heterostructures. The surface reactions occurring at the Si-metal interface and the state of the graphene layer were revealed continuously while intercalating up to 4-5 monolayers of Si below graphene. For both systems we found that Si atoms do not simply accumulate on top of the substrate but intermix with it in a complex sequence of competing processes. By simultaneously monitoring the metal-Si interface and the graphene layer by core level spectroscopy we could establish how the subsequent interface configurations relate to the charge transferred to graphene and determine how the graphene doping level depends on the amount of intercalated Si.

Intercalation of oxygen below Gr/Si/metal leads to the synthesis of ultrathin  $\text{SiO}_2$  layers below graphene [2]. The intercalated oxygen modifies the metal-oxide work function and acts as a stable and durable mean to hole dope graphene. We show that the Gr| $\text{SiO}_2$ |metal heterostructure behaves as a gated plane capacitor with the oxide layer acting as a homogeneous dielectric spacer. The hole doping, obtained without the need to include heteroatoms in the honeycomb lattice or adsorbates on top of it, can be tuned by controlling the amount of the interfacial oxygen, as well as by adjusting the thickness of the oxide layer. The evidence that good quality graphene can be grown on metal thin films discloses the possibility to extend this approach substituting single crystal substrates with low-cost thin metallic layers.

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**#612 - Applications of light-activated nano-gold and graphene in therapy, drug delivery and sensing***Roberto Pini (I) - Istituto di Fisica Applicata "Nello Carrara" - CNR**Other Authors: Paolo Matteini, Fulvio Ratto, Francesca Rossi, Marella de Angelis, Martina Banchelli, Lucia Cavigli, Sonia Centi, Francesca Tatini Istituto di Fisica Applicata "Nello Carrara" - CNR*

Nanophotonics solutions are providing new answers to topical biomedical challenges. A relevant example is the use of laser-activated plasmonic nanoparticles and graphene for generating heat or for enhancing the local electric field. These processes are being exploited for a variety of biomedical applications including cancer therapy, tissue repair, drug delivery and biosensing. Here

we will present into more details some light-activated materials, which we have recently developed and proposed as viable solutions to critical issues in therapy and sensing applications.

A first example is the combination of pulsed and CW near-infrared laser light with plasmonic particles such as gold nanorods is gaining relevance for the photoacoustic imaging and photothermal ablation of cancer. Selective targeting of malignant cells with these contrast agents may rely on complementary biochemical and biological strategies, including the use of specific probes or the exploitation of cellular vehicles. Here we moved from a platform of PEGylated gold nanorods with plasmonic bands around 800 nm, good biological profiles, stability and efficiency of photoacoustic and photothermal conversion as well as potential to passively accumulate into solid tumors by their enhanced permeability and retention. In vitro studies on cell cultures on those different approaches will be presented and discussed.

For drug release, nano-gold and other light-responsive nanometaterials can be employed for the development of an implantable device for on demand chemical release in the form of a light-activated sponge-like scaffold. The photothermal response of the gold nanoparticles contained inside the sponge triggers a contraction in proximal drug-loaded thermosensitive micelles, thus promoting the expulsion of the drug from the sponge. An advanced version of this devices consists in a dispersion of graphene nanosheets in a biopolymer matrix, which is activated by millisecond-long light pulses for confined and precisely dosed drug release.

Finally examples of the potential of organized bidimensional assemblies of gold and silver nanocubes decorated with a graphene film will be described for the direct Surface Enhanced Raman Scattering (SERS) analysis of proteins and biomarkers. In this regard, we will introduce a SERS sensor we engineered for the rapid and reproducible quali-quantitative detection of toxic amyloid oligomers associated with neurodegenerative diseases.

### #613 - Temperature Influence of Production of Single and Multilayer Graphene Oxide

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Since Andre Geim and Konstantin Novoselov were awarded the Nobel Prize for their groundbreaking experiment regarding the two-dimensional material graphene[1], carbon allotrope materials have attracted the interest of the research community[2,3]. Recently, graphene (single) and graphite (multilayer) oxide, have been considered to be a promising material in a wide scenarios of emerging technologies due to their properties, as well as, for their low production costs. Our investigation is focussing on modulating the properties of oxidized carbon materials modifying the initial synthetic conditions in the view of applications based on nanotechnology such as sensors or hydrogen storage substrates[4]. By using a few-steps method two forms of graphene oxide are generated, i.e. single or multilayer, which depends on the operating temperature. Even if apparently similar, these materials exhibit distinctive physical and chemical properties with a distinct reactivity which affects the characteristic of a possible future applications. Archived behaviour suggests a scenario where the properties needed for a device can be straightforward obtained by changing the temperature. Moreover, the final oxidized product acquired a variation in the behaviour when another carbon allotrope (single wall material) is employed as a reagent. Those materials gather the prospect of an advantage owing to the feasibility of modulate/engineering the properties and the low cost and scale up production.

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### #614 - Scanning Auger Micro-spectroscopy for thickness evaluation of Graphene and Graphene Oxide layers

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Graphene is the archetype 2D material, and its unique properties widely appeal to applications, from electronics, to energy storage, photonics, composite materials and sensor technology. Graphene oxide (GO) can be easily dispersed in solvents and deposited with controlled thickness onto different substrates. Because of the variety of its oxygen-functional groups, GO can interact with wide range of organic and inorganic materials. Since it is tunable from insulator to semi-metal, it is promising for applications such as plastic electronics, solar cells and biosensors. As is in general for 2D materials, the physical properties of graphene and GO crucially

depend on the number of stacked atomic layers composing the film. It is therefore of the utmost importance to quantify the number of layers and the overall thickness of the films obtained from different growth processes. Nanoscale thickness metrology techniques are possible, like atomic force microscopy (AFM), optical microscopy, contrast spectroscopy, confocal Rayleigh scattering microscopy and micro-Raman ( $\mu$ -Raman) spectroscopy. Among these, AFM and  $\mu$ -Raman spectroscopy directly identify the number of layers. However, depending on the substrates, Raman technique may not be applicable and AFM is mainly limited by the small field of view and the need for a step-shaped sample to refer to substrate for levelling. Recently, Scanning Auger Microspectroscopy (SAM) has been demonstrated to be sensitive for thickness measurements of graphene layers on silica substrates. We extend SAM characterization to generic substrates and to GO, by evaluating reference layer number by AFM and  $\mu$ -Raman, where applicable, and by overcoming the limitations of AFM and  $\mu$ -Raman themselves. Firstly, updated values for the electron effective attenuation lengths in graphene and GO were experimentally determined with unprecedented accuracy, for each film/substrate combination. Then, the absolute thickness of graphene and GO flakes, up to 4 monolayers thick, was evaluated by SAM; results are consistent with AFM and Raman measurements, with a standard deviation well below a single monolayer. SAM, associated with SEM imaging, represents a method for quantitative thickness mapping of large area graphene and GO films and related devices with sub-monolayer resolution. This method is capable of detecting chemical impurities, on a very wide variety of substrates, from conductors to insulators and from heavy to light atomic weight compounds.

### #615 - Behavior of the Berry phase in gapped graphene

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Using a minimal tight-binding model, we show that when a gap of tunable size opens at the conic band intersections of graphene, we show that the Berry phase in graphene does not vanish abruptly, but progressively decreases as a function of the gap. or more precisely of the extension of the quadratic-dispersion region around the former Dirac point. The phase now depends on, and increases with, with the radius of the path in  $q$ -space: when electrons are doped into the system, that radius is just the Fermi wave vector, which obviously can be directly tuned. It follows that the Berry phase and its observable consequences can be tuned away from their value in graphene by tuning the gap by a modulating potential through shear-including strain or nanostructuration, and adjusting the doping level. Transport properties (such as the Klein paradox) related to chirality conservation should also behave accordingly.

### #616 - Plasmon losses in monolayer graphene

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Graphene sheets encapsulated between hexagonal Boron Nitride (hBN) slabs display superb electronic properties due to very limited scattering from extrinsic disorder sources such as Coulomb impurities and corrugations. Such samples are therefore expected to be ideal platforms for highly-tunable low-loss plasmonics in a wide spectral range. We present a theory of collective electron density oscillations in a graphene sheet encapsulated between two hBN semi-infinite slabs (hBN/G/hBN). Graphene plasmons hybridize with hBN optical phonons forming hybrid plasmon-phonon (HPP) modes. We focus on scattering of these modes against graphene's acoustic phonons and hBN optical phonons, two sources of scattering that are expected to play a key role in hBN/G/hBN stacks. We find that at room temperature the scattering against graphene's acoustic phonons is the dominant limiting factor for hBN/G/hBN stacks, yielding theoretical inverse damping ratios of hybrid plasmon-phonon modes of the order of 50-60, with a weak dependence on carrier density and a strong dependence on illumination frequency. We confirm that the plasmon lifetime is not directly correlated with the mobility: in fact, it can be anti-correlated. Finally, we compare the plasmon losses due to the electron-phonon scattering with those due to electron-electron and electron impurity interactions. We demonstrate that graphene's sublattice-pseudospin degree of freedom suppresses the electron-electron plasmon losses with respect to those that occur in ordinary two-dimensional electron liquids.

**#617 - Adaptive Soft Matter: from self-structuring to optical materials**

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Collective effects in ensembles of microscopic particles or molecules drive many processes in nature and can be exploited in designing complex functions in macroscopic systems. Among others, light activated molecular switches are a particularly interesting case, since they can be remotely addressed by light of suitable wavelength or power. In the last twenty years, azobenzene molecular units have attracted interest due to the possibility of switching the molecule from a trans- to a cis-isomer (and back to trans-) by illuminating it with light in the visible spectral region.

Consecutive trans-cis-trans photo-isomerization cycles can be induced with a final orientation of the molecules perpendicular to the light's polarization direction. This has triggered applications in holographic data storage. Furthermore, the difference in length (around 0.4nm) between the azo-units of the two photo-switchable isomers has allowed their use as molecular photo-activated nano-actuators.

When the azo-units are embedded (usually as side chains) inside a polymeric matrix, another collective effect of the light-induced isomerization is the modulation of the polymer surface according to free energy minimization and total volume conservation. Complex morphologies can be obtained by exploiting this effect; this is, in fact, a photo-lithographic mechanism for the polymer surface. The unique photo-response of azo-polymers allows developing a new photo-lithography platform where the optical field distribution is engineered to achieve complex, large-scale and high-resolution patterns, overcoming the resolution limit of conventional photo-lithography.

**#618 - Measure on intracellular chloride in the brain by means of non linear microscopy**

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Brain computations is due to the concerted activity of cortical neurons. In its simplest form, neuronal activity is the product of the integration of excitatory inputs coupled to an inhibitory feedback that curtails excessive excitation, keeping the system within the allowed dynamic range. Any disturbance of the dynamical equilibrium between excitation and inhibition invariably leads to a pathological state of the brain network. Recent years have seen the exploration of these processes in the intact brains by means of two photon microscopy and by fluorescent tools which optical properties depends on intracellular environment. This advancements allows to visualize simultaneously the activity of several neurons in the intact brain.

We are studying the excitation/inhibition feedback by looking at the very basis of inhibitory synaptic transmission. This is brought about by the release at inhibitory synapses of the neurotransmitter Gamma Amino Butyric acid (GABA). GABA binds to its receptor causing the opening of a channel mainly permeable to chloride. The resulting current changes the intracellular membrane potential. In the healthy, adult cortex, intracellular chloride is very low compared to the extracellular media, thus chloride flows in and this current inhibits the neuron by shifting the intracellular potentials towards negative values. In contrast, in the immature brain and in a variety of pathologies, it is believed that intracellular chloride is quite high. In this conditions, the activation of GABA receptors has a paradoxical effect letting chloride out of neurons and thus facilitating neuronal excitation. Thus, the regulation of intracellular chloride has an obvious importance, but, notwithstanding 20 years of efforts, it has not been possible yet to measure intracellular chloride *in vivo*.

Here, we have devised a method for absolute measurement of chloride (and pH) *in vivo* in rodents by using a genetically encoded sensor formed by the fusion between a chloride and pH sensitive GFP ( $E^2$ GFP) and an insensitive RFP (msKate). First, we characterized the 2-photon spectral properties of the sensor, showing that increasing chloride causes a decrease of the green/red fluorescence. A shift in pH causes a strong alteration of the 2-photon excitation spectra of  $E^2$ GFP. Then, the sensor was targeted to the mouse sensory cortex by means of *in utero* electroporation. We demonstrated the integrity and stoichiometry of the sensor by *in situ* fluorescence correlation spectroscopy and by measuring trafficking across the nuclear membrane. Then, we found that brain tissue has a strongly wavelength-dependent effect on the propagation of excitation and emission strongly affecting the pH and Chloride measures. By means of analytical spectral decomposition we could measure and compensate for the spectral distortion caused by the tissue. Our data are the first direct measure of intracellular chloride *in vivo*.

**#619 - Luminescence and sensing properties of N-rich Carbon dot as a function of nitrogen content.**

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The optical properties of carbon dots (CDs) are undoubtedly the main motivation currently driving a lively research on this new family of carbon-based nanomaterials, together with their biocompatibility, absence of toxicity, and easy preparation. Besides, the intense luminescence unquestionably makes CDs an actual functional material, with a great potential in important applications such as sensing of metal ions. Doping is the main technique to tailor the defects, impurities, electrical, and emission properties of C-based nanomaterials; for this reason, Sulphur-Nitrogen co-doped CDs and Boron- or Nitrogen- doped CDs have been reported lately in the literature, showing very high fluorescence quantum yield (from 28 to 78%).

Nitrogen is found to enhance the fluorescence quantum yield of CDs and to provide them with peculiar optical properties. Hence in this work, a protocol to carry out the microwave preparation of CDs with different contents of Nitrogen atoms is developed, and a study to correlate their luminescence properties to the N-content is reported. Two emission signals are detected and correlated to the amount of dopant. In order to investigate the functional properties of these N-rich Carbon Dots, we also tested their behavior as sensors for metal cations such as Cu(II), whose working principle exploits the interactions between surface moieties of CDs and cations.

#### #620 - Au nanostructures on a large area: optical and functional properties for chemical sensing

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There is great interest in assembling gold and silver nanoparticles (NPs) onto flat substrates for investigating Localized Surface Plasmon resonance (LSPR) - based phenomena. The unique optical properties of metal nanostructures, that are absent in the bulk or flat surfaces, give rise to intense absorption bands, with their intensity and position depending markedly on the size, shape, distribution and on the refractive index of the environment surrounding the nanoparticles, as predicted by Mie Theory[1-2]. These properties makes the metal nanostructured interfaces suitable transducers for gas or bio-sensing applications by monitoring the change in the refractive index due to the liquid or gas-surface interaction taking place onto the surface of the metal nanoparticles.

The use of LSPR- based phenomena for chemical and biological sensing is of special interest, because it allows the label-free detection of extremely small concentrations of target molecules. Due to relatively short ( $\approx 30$  nm) electromagnetic field decay length of the metallic nanoparticles, their surface sensitivity is much higher, in comparison to that of flat SPR sensors, using thin metallic films as transducers.

In this work, the results achieved in this field by the optical sensor group of CNR-IMM Lecce are presented. In particular, the different strategies adopted for the realization of Au NPs over large areas of glass substrates with physical and chemical preparation techniques are presented and compared. Optical properties of the realized nanostructures are related to their shape and distribution both in a two-dimensional and three dimensional configuration.

Modelling tools, supported by morphological and structural information, will help to predict and realize a proper design of the investigated materials tailored on the nanoscale. Optical and morphological properties will be correlated with functional properties of the realized nanostructures by showing how they can be used as a proper transducers for optical chemical and biosensors and the strategies chosen for improving their sensing performances.

Finally, a new sensing probe based onto magneto-optical properties of the realized structures will be proposed and presented. In particular, the interaction between the electronic oscillations of the metal nanostructures and a magnetic field of low intensity applied in a proper configuration will be demonstrated and discussed.

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#### #621 - Ultrastrong light-matter coupling in electrically doped microcavity organic

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The coupling of the electromagnetic field with an electronic transition gives rise, for strong enough light-matter interactions, to hybrid states called exciton-polaritons. When the energy exchanged between light and matter becomes a significant fraction of the material transition energy an extreme optical regime called ultrastrong coupling (USC) is achieved. We report a microcavity embedded p-i-n monolithic organic light emitting diode working in USC, employing a thin film of squaraine dye as active layer. A normalized coupling ratio of 48% has been achieved at room temperature. These USC devices exhibit a dispersion-less angle-resolved electroluminescence that can be exploited for the realization of innovative optoelectronic devices. Our results may

open the way towards electrically pumped polariton lasers

### #622 - Biomorphic Optical Functions in Vegetable Seeds

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Biophoton emission has been largely investigated during the last century. It was reported with different names, ranging from biophotons to dark-luminescence, to ultraweak light emission and so on... All such names describe the capability of biological structures to emit light in specific environments or when the biological structures are somehow stressed.

Here we report biophoton emission from germinating seeds (more specifically cannellini beans). Analysis of emitted luminescence during imbibition by "vital" as well as "denaturated" parts of seeds points out both coherent and incoherent statistics of photons. Each behaviour was reproducible in all analysed samples.

Is there any specific reason for such light emission? Is it just a chemical "waist", a funny phenomenon or it is functional for the vital life of the seed and the future plant? Starting from the very general opinion that nature does nothing without reasons, we have analysed cannellini beans from the optical point of view. We consider seeds as close envelopes, partially filled by cotyledons.

Geometrical and optical analysis of seeds as resonators, using a ray-tracing protocol, have pointed out proper optical functionalities of the morphology which are crucial for the internal regulation of the germination process.

Numerical predictions have been experimentally confirmed by internal photon-counting measurements during germination.

### #623 - Recent advancements in design and characterization of Yb-doped transparent ceramics for high power laser applications

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Ceramic-based materials provide a viable alternative to single crystal materials as active media for solid state lasers.

The ceramic process is highly flexible in terms of possible geometries and shapes, as well as dopant distribution control and allows to build innovative structures which are currently unfeasible with the crystal growth technology, but can be very useful for high power applications.

A key aspect in the design and operation of high power laser devices is the management of the thermal effects (TEs) and thermo-mechanical effects (TMEs) (e.g. thermal lens, stress-induced depolarization, surface deformations) deriving from the laser pumping process, which degrade the performance of the laser source and can eventually lead to a catastrophic failure of the laser active element. In this communication we enlighten our recent advances in the design, fabrication and characterization of laser ceramics based on Yb doped YAG.

The issues related to the design, the production process and the characterization of the laser emission properties were investigated. Moreover, different fabrication methods suitable for the realization of complex shapes and structured doping (with non-uniform dopant distribution) were tested and compared.

Planar structures of Yb:YAG with longitudinal distribution of Yb concentration were designed and optimized by means of Finite Elements Analysis, for the evaluation of their thermal and thermo-mechanical behavior under various pumping and cooling geometries. Suitable non-uniform doping distributions were effective for the mitigation of the internal thermo-mechanical stress and the reduction of peak temperature, with respect to structures with homogeneous doping.

Two different fabrication processes were compared, the so called tape casting technique followed by thermal compression, and the cold pressing of spray dried powders. The microstructure of the ceramic elements and the Yb concentration profile across the interfaces of regions with different doping have been characterized by FEG SEM and ESEM equipped with EDS.

The laser behavior of the samples has been analyzed in a longitudinally diode pumped laser cavity under high intensity power pumping, under different thermal load conditions. The laser efficiency under high thermal load conditions has been compared to that obtained from samples with uniform doping, under the same test conditions.

**#624 - Synthesis of Graphene Nano-Ribbons by Surface Polymerisation of Molecular Precursors**

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Size confinement of graphene can generate an energy gap [1], a fundamental step towards its utilisation in several technological applications. To this end, synthesis of sub-nanometer-wide Graphene Nano Ribbons (GNR) with atomically controlled shape and width can be obtained by adsorption of molecular precursors on metal surfaces, followed by thermal activated chemical reactions [2].

In this work, a high-resolution spectroscopic study of 10,10-dibromo-9,9 bianthracene (DBBA) molecules deposited on the Au(110) surface is presented, by means of high-resolution ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS), and X-ray absorption spectroscopy (XAS) [3]. Through the thermally activated procedure, these molecular precursors polymerise and eventually form GNRs. We follow all the different steps of synthesis by high-resolution UPS and temperature-programmed XPS, which brings to light the chemical modifications from molecular dehalogenation to polymerisation and eventual formation of the typical C-C bonds of GNR, and by XAS with linearly polarised radiation, allowing to determine the flat orientation of the achieved graphene nanostructures.

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**#625 - Molecular orbital mapping of organic semiconductors at the molecular/metal interface**

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Thin film organic semiconductors have many prospective applications for developing low-cost and robust devices, which can fill niches not occupied by silicon-based electronics. Organic molecules such as phthalocyanines (Pc) and tetracyanoquinodimethane (TCNQ) deposited on the surface have a tendency to self organize and form highly ordered patterns, making them attractive for technological applications in colorimetric gas sensors, photonic wires, field-effect transistors, light emitting diodes, catalysts, optical switches and data storage []. Recently, it was shown that organic semiconductors have a great opportunity for application in the growing area of spintronics, where active manipulation and control of the electronic spin degree of freedom are of interest. For example, the interaction of TCNQ with transition metals (TM) has a tendency to form coordination networks exhibiting interesting magnetic properties, and the magnetic properties can be controlled by employing different combinations of the TM atoms.

We have carried out a comprehensive study of the adsorption behavior of FePc, TCNQ and Mn-TCNQ on the low-index crystal faces of silver and copper. Experiments were carried out at the NanoESCA beamline of the Elettra synchrotron [1]. The experimental setup includes a non-magnetic, electrostatic photoelectron emission microscope (PEEM) and a double-pass hemispherical analyzer directly images a parallel momentum component of photoelectron at a fixed binding energy. A combination of photoelectron momentum mapping (PMM) and low-energy electron diffraction (LEED) and theoretical modelling provides access to the superstructure unit cell and the arrangement of the molecules within the unit cell. Additionally, momentum patterns give information about the electronic structure at the interface and the symmetry of molecular orbitals. An analysis of the PMM of the lowest unoccupied molecular orbitals (LUMO) of FePc on the substrates with different symmetry indicates that both degenerate LUMOs receive charge transfer from the substrate [2]. On the Ag(100) substrate, TCNQ forms two superstructures depending on the density of molecules on the surface. The co-adsorption of Mn metal leads to formation of a new ordered metal-organic coordination network [3].

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### #626 - Self assembly properties and electronic excitations of organic thin films explored by synchrotron based core-electron spectroscopies.

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Synchrotron radiation-based techniques are powerful tools for determining the crystallographic and electronic structure of organic thin films. In particular, high-resolution photoemission spectroscopy (XPS) and polarization-dependant near edge X-ray absorption fine structure (NEXAFS) provide valuable information on the structural conformation of the molecular constituents as well as on the chemical interaction and charge transfer at the organic/inorganic interface. Here the application of synchrotron-based core-electron spectroscopies is shown for two organic systems exhibiting completely different levels of hierarchical self-assembly: eumelanin thin films and donor-acceptor molecular monolayers. In the highly disordered eumelanin compound, the chemical composition, aggregation behavior and electronic properties of eumelanin molecular building blocks are revealed on the base of polarization-dependant NEXAFS measurements [1]. In crystalline donor-acceptor monolayers deposited on noble metal (111) surfaces, the hole injection barriers and interfacial charge transfer are determined by a powerful combination of surface sensitive techniques [2]. It is unraveled that the formation of an ordered mixed layer with a maximized donor-acceptor contact area leads to a characteristic energy level alignment at the molecule/metal interface regardless of the particular molecules and substrate. The possibility to trigger charge transfer into empty molecular levels by choosing the appropriate supramolecular architecture is also established.

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### #627 - Interface Local Structure in Chalcogenide Superlattices

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Summary. *The structural properties of the Ge-Te-Sb interface in interfacial phase change materials (iPCMs) is studied by EXAFS experiments at the Ge and Sb K-edge, supported by TEM measurements. Based on this analysis, we propose a new structure, where 3Ge-Te layers are inserted into 1Sb<sub>2</sub>Te<sub>3</sub> QL and the Sb layers in this building-block present an intermixing with Ge atoms.*

The need of fast and efficient management of information stimulates research on active materials with tunable properties. Phase-change materials (PCMs) are representative compounds, exploiting the exceptional properties of chalcogenide glasses for memory device applications. [1] A PCM is identified by its ability of switching reversibly between a high-conductive crystalline state and a low-conductive amorphous state, via an atomic movement involving a melted metastable state. The phase transformation is in general triggered by electric current or light pulses of different time duration and amplitude.

Most PCMs are alloys constituted by mixtures of Ge, Sb and Te elements, the so-called GSTs, but there is continuous effort to develop novel compounds with improved performances. [2] Within this framework, the class of interfacial phase-change materials (iPCMs) was designed. [3] They theoretically present a superlattice (SL) structure of alternating GeTe(111) bilayers and Sb<sub>2</sub>Te<sub>3</sub>(001) quintuple layers, well separated by van der Waals gaps. The SLs are characterized by the ability to switch without melting, thus resulting in a confined short-range atomic movement. iPCM are shown to function with lower power threshold and faster switching time. [3]

Therefore, the crystalline structure of iPCM must be studied in detail. Various models are proposed in literature [4], but limited and controversial structural investigations on high quality SL are available. On this purpose, we performed Extended X-ray Absorption Fine Structure Spectroscopy experiments at the Ge and Sb K-edges on very high quality samples grown by state-of-the art molecular beam epitaxy (MBE) technique. EXAFS signals at the Ge (11.1 keV) and Sb (30.5 keV) K-edges were collected at the SAMBA beamline (Synchrotron SOLEIL). Data analysis and fitting were carried out by means of Ge and Sb K-edges co-refinement procedure using ARTEMIS code [5], and by a Morlet wavelet transform analysis [6].

The present work reveals non sharp separation at the GeTe/Sb<sub>2</sub>Te<sub>3</sub> interface in ultra-thin Ge-Sb-Te based superlattices. The interface local atomic structure in the proximity of the Van der Waals gap and the Sb/Ge intermixing are reported and discussed.

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**#628 - Numerical simulation for Space-Charge effect in Photoemission experiments with ultrashort sources.**

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The availability of lasers and Free Electron Lasers (FEL) allows in principle to perform time resolved photoemission experiments for studying the dynamics of electronic structure evolution of materials [1,2,3].

Both sources are characterized by high peak powers and therefore a large number of photoelectrons are emitted in very short time intervals.

In these conditions the mutual Coulomb interactions (space-charge effect) generate shift and broadening of the energy spectrum of the photoelectrons that can obscure the physical meaning of the measures.

Therefore it is of primary importance to have effective methods of prediction of these effects in order to determine the measurement conditions that minimize the distortions of the spectrum.

In this work we present a comparison between two different numerical simulation approaches, stochastic and deterministic.

The stochastic approach solves the Poisson equation and is used by SIMION [4], the deterministic one takes in to account the individual repulsion among the electrons through Treecode [5].

We have tested the accuracy of a widely used tool, such as SIMION, for predicting the energy distortion caused by the space-charge effect in any type of analyzer.

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**#629 - 3D Coherent Diffraction Imaging with hard X-rays applied to the study of giant photoluminescence emission in porous nanoparticle Si layers**

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Coherent X-ray diffractive imaging (CXDI) is a novel lens-less scattering technique [1,2] that exploits the unprecedented degree of coherence of modern synchrotron sources. It has potential for high resolution imaging of isolated microscopic objects beyond the values achieved with X-ray optics and represents an interesting tool to bridge the gap between high resolution electron and visible light microscopy. The image in the real space is obtained by applying a phase retrieval algorithm to the diffraction pattern measured with sufficient oversampling. Because of the high penetration power of the X-rays the imaging of thick object (<10micron) without sectioning is possible in 3D [3,4,5].

Here we report about the current status of 3D CXDI at the ESRF beamline ID10. We discuss the possibilities and challenges of CXDI by presenting an example of 3D reconstructions of porous Si clusters made of different nanoparticles. The high quality of the reconstructed images reveals individual Si nano-crystals and allows studying the role of the porosity in the stimulated giant photoluminescence emission [6].

The development of large 2D (pixel) detectors is the key element for achieving the full potential of the technique.

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**#630 - Matter Under Extreme Pressures**

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High pressure physics, in the Mbar range, is a broad, and rapidly developing field, which requires state (and beyond)-of-the-art experimental technologies such as the diamond anvil cell, laser heating, dedicated optical spectroscopies, and synchrotron methods. I will briefly review some results through the years on remarkable, pressure induced phenomena, such as the insulator-to-metal phase transition in simple molecular systems [1,2], the metal-to-insulator phase transition observed in alkali metals [3,4,5], liquid-

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liquid phase transformations or transitions [6], gas like-to-liquid like dynamical and thermodynamical crossovers in supercritical fluids [7,8], along with the synthesis of new materials [8,9,10]. Finally, I will introduce the warm dense matter state in the hundred Mbar/Gbar range and how this largely unknown state could be produced and investigated, *in situ*, by using laser induced shock-waves combined with synchrotron based, material characterization techniques.

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# Posters

**#P001 - Hot Electron Production and Characterization in SI-relevant Regime**

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Shock ignition (SI) [1] is a novel approach to (ICF) [2], based on the separation of the compression and ignition phases of a DT pellet. The first one is driven by ns laser beams at  $I < 10^{15} \text{W/cm}^2$ , the second with ps laser intensities  $I \approx 10^{15} - 10^{16} \text{W/cm}^2$ . At such intensities, laser interaction with the long scalelength plasma may lead to the generation of hot electrons (HE). Our experiment aims at investigating the generation of such HE and their role in the generation of the shock wave[3]. We used two beams of the iodine laser PALS: an auxiliary beam ( $1\omega$ ) (60 J,  $1 \times 10^{14} \text{W/cm}^2$ ), and a main beam (wavelength  $\lambda = 1315/438 \text{ nm}$  for  $1\omega/3\omega$ , respectively, pulse duration  $\approx 0.3 \text{ ns}$ , energy between 170 and 440 J focused to intensities up to  $I = 2 \times 10^{16} \text{W/cm}^2$ ). The auxiliary beam arrived on target up to 1.2 ns before the main one, simulating the long-scale pre-plasma typical of ICF. Then the main beam was used to launch a strong shock.

We used different targets: plastic+Ti+Cu, plastic+Cu+Al, pure Cu. The preplasma originated from plastic ( $\text{C}_6\text{H}_7\text{Cl}$ ) where Cl atoms allowed using X-ray spectroscopy to get plasma temperature. Hot electrons were detected by K-emission from the Cu and Ti layers. The measured K- $\alpha$  size was  $\approx 100 \mu\text{m}$ . By simulating hot electron propagation and K-shell emission inside the studied targets with GEANT4 and PENELOPE we could infer a laser-to-electron conversion efficiency  $\eta \approx 0.65\%$  and an average hot electron temperature  $\approx 30 \text{ keV}$ .

**#P002 - Study of the self-modulated propagation of relativistic charged particle beam in warm-magnetized plasmas, within the kinetic description**

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An investigation of the self-modulation of a charged-particle beam in a plasma, while experiencing the plasma wake field self-interaction, is carried out within the kinetic description. The beam is assumed to be relativistic and of arbitrary length. On the other-hand, the plasma is warm, externally magnetized and collisional. Stability analyses of the "beam-plasma" system, including suitable stability criteria, are also provided.

**#P003 - Luminescent proprieties of a Metal-Organic Framework: Al-fumarate**

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Metal-organic frameworks (MOF) are a new class of materials which are evoking a remarkable interest in Science for their peculiar proprieties. They are regular three-dimensional polymers consisting in a network of metal ions connected by organic linkers. The most important propriety of MOFs is their ability to adsorb ions or molecules within a pattern of regular cages made available by their extraordinarily porous structure. In addition, their synthesis can be widely tailored to confer them with very flexible structural proprieties. Beside porosity, many MOFs can have luminescent proprieties which can be used in different technological fields like sensing, tunable light sources, and drug delivery.

Here we report a study of the luminescence properties of a specific MOF of recent discovery, Al-Fumarate, one of the few examples of Aluminum-based MOFs. The structure of Al-Fumarate can be pictured as a regular network of Al(III) ions connected by fumarate ( $\text{C}_4\text{H}_4\text{O}_4$ )<sup>2-</sup> linkers. The main benefits of Al-fumarate are its stability in aqueous environment, which hinders practical applications of many other MOFs, ease of production and low cost, combined with a remarkable porosity (surface area  $\sim 1000 \text{ m}^2/\text{g}$ ) deriving from a regular one-dimensional structure of channels. Our study of Al-fumarate by time-resolved photoluminescence spectroscopy led to observe an emission band peaking at  $2.74 \pm 0.03 \text{ eV}$  when exciting the sample at  $3.54 \text{ eV}$ . The room-temperature decay kinetics of this signal is a stretched exponential with  $\tau = 2 \text{ ns} \pm 0.2 \text{ ns}$  and stretching parameter  $B = 0.6 \pm 0.02$ . Notably, we find that the photoluminescence of Al-fumarate is tunable, in that its emission peak continuously shifts with the optical excitation energy. This property, combined with the non-exponential decay kinetics, reveals a remarkable degree of disorder of the system despite its well-defined crystalline structure. Temperature-dependent luminescence experiments also allowed us to disentangle the radiative and non-radiative contributions to the luminescence decay. Overall, the experimental data provide an extensive picture of the optical properties of Al-fumarate, which may have an impact on future applications of this MOF.

**#P004 - Similar structural dynamics for the CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> degradation in air and vacuum**

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Lead iodide perovskites have been raising a large attention due to their structural peculiarities and the intriguing transport capabilities. The easy preparation procedure and the competitive electrical behaviour have been pushing forward a rapid development of solar cells based on perovskite-like materials towards record efficiency values (above 20%). Nevertheless, structural stability and degradation issues still remain main concerns that are not fully explored. Their deep knowledge is nowadays mandatory to define proper strategies for a large durability of the photo-active material.

Lead iodide perovskites are unstable especially under air/moisture exposure, which causes degradation towards lead iodide. PbI<sub>2</sub> inclusions in the cell architecture are indeed detrimental for the cell parameters and performances, and therefore some strategies to protect the perovskite layers against ambient exposure have been proposed, (e.g. by Al<sub>2</sub>O<sub>3</sub> or polymeric coatings).

We thus investigate the degradation path of methylammonium lead iodide (MAPbI<sub>3</sub>) films over flat TiO<sub>2</sub> substrates at room temperature by means of X-Ray Diffraction, Spectroscopic Ellipsometry, X-ray Photoelectron Spectroscopy and High Resolution Transmission Electron Microscopy.

We find out that the degradation dynamics is similar in air and vacuum conditions; thereby the water molecules action is not the unique source of instability. We argue that the degradation process has, in both cases, an early stage, which drives the starting tetragonal lattice in the direction of a cubic atomic arrangement, at fixed MAPbI<sub>3</sub> stoichiometry. Such early stage is followed by a phase change with the PbI<sub>2</sub> as the main solid product. This degradation product is structurally coupled with the original MAPbI<sub>3</sub> lattice through the orientation of its constituent PbI<sub>6</sub> octahedra and progressively erodes the starting MAPbI<sub>3</sub> film.

The similarity of the degradation dynamics in air and vacuum highlights the occurrence of intrinsic thermodynamic mechanisms not necessarily linked to humidity.

**#P005 - Modeling and Development of a Double-Tuned (23Na/1H) Birdcage RF Coil for 2.35T Magnetic Resonance Imaging Biomedical Applications**

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Magnetic Resonance Imaging (MRI) is proving to be a very useful tool for proton and sodium quantification in animal models of stroke, ischemia, and cancer. For example, sodium MRI was able to monitor chemotherapeutic response in rat glioma models [1]. To this purpose, specially designed double-tuned RF coils are required and many design configurations have been described in the literature [2-3].

In this work, we present the modeling and development of a dual-frequency RF volume coil suitable for <sup>1</sup>H and <sup>23</sup>Na images of small/medium size samples at 2.35T, made by two coaxial birdcage coils.

A numerical FEM method (HFSS 15.2; eigenmode model; double 6128AMD Operon at 2GHz, 16 cores, 28GB of RAM to run the simulation) was used to model and optimize the RF coil, taking into account the ratio between the coils diameter and length. We also considered the effect of the RF shield on B<sub>1</sub> field intensity and homogeneity. Linear driving of the two channels and a careful angular orientation between the coils minimized the mutual coupling between the <sup>1</sup>H and <sup>23</sup>Na coils.

The current configuration of the dual-frequency RF coil is made of two coaxial birdcage coils: i) a larger (diameter 105 mm, length 160 mm) high-pass birdcage coil comprising 8 copper legs (5 mm width; 35 μm thickness) tuned to the <sup>1</sup>H frequency (100.3 MHz); and ii) a smaller (diameter 90 mm, length 130) low-pass birdcage coil comprising 8 copper legs (5 mm width; 35 μm thickness) tuned to the <sup>23</sup>Na frequency (26.6 MHz). The RF shield is selected with diameter 151 mm and length 210 mm. Without RF shield the coil set was tuned at 2.35T by using <sup>23</sup>Na and <sup>1</sup>H capacitances, respectively, of 385pF and 49pF. In the presence of the RF shield the resonant frequencies of the <sup>23</sup>Na and <sup>1</sup>H coils increase, respectively, of about 10% and 7%. In this condition, the coil was retuned by increasing the <sup>23</sup>Na and <sup>1</sup>H capacitances, respectively, to 480pF and 52pF. Work is in progress to build a prototype suitable for workbench and MRI testing with phantoms and small laboratory animals (mice/rats).

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**#P006 - Point-Of-Care Plastic Biosensor Devices using a PEDOT-modified Electrochemical Glucose Sensing Platform**

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There is an emerging global epidemic of diabetes that can be related to rapid increases in overweight, including obesity and physical inactivity. According to World Healthcare Organization, diabetes is a leading cause of blindness, amputation and kidney failure, while total deaths from diabetes are projected to rise by more than 50% in the next 10 years. To prevent life threatening and debilitating complications associated with diabetes, researchers are continuously involved in developing glucose biosensors. Hence, it is essential to develop a biosensor that can determine glucose levels having fast-response, high sensitivity and selectivity. Depending upon the transduction technique, a number of glucose biosensors have been reported, including electrochemical, optical, and electromagnetic spectroscopy biosensors. Among these types, electrochemical biosensors have been most widely accepted for the sensitive detection of glucose.

Electrochemical biosensors offer an attractive opportunity for quick and sensitive detection of analytes in blood. In the present work, polymer, namely poly(3,4-ethylenedioxythiophene) (PEDOT), films have been electropolymerized on Au electrodes on polyethylene terephthalate (PET) substrates. Glucose oxidase (GOx) enzyme was immobilized on the PEDOT films via glutaraldehyde chemistry. These fabricated plastic biosensors exhibited a high sensitivity of  $7.4 \text{ mA}/(\text{mM}\cdot\text{cm}^2)$  over the clinic range (2-10 mM) of glucose by employing a low cost technology. The biosensors were coupled with an electronic interface just to show the possibility to easily integrate such devices with the emerging technologies including those of smart phones or other wireless based systems able to assist patients in remote. The potential to use our systems for sensing different analytes for a wide range of applications will be discussed. Elettronica su plastica per sistemi " smart disposable" project under PON 2007-2013 program is acknowledged.

#### #P007 - Radiative properties of multisubband plasmons in semiconductor quantum wells

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Plasmonic excitations are ordinarily associated to intraband transitions in metal-like electronic systems dressed by the mutual Coulomb interaction [1]. A quasi-two-dimensional electron gas with multiple subbands, such as a highly doped semiconductor quantum well, presents additional plasmonic excitations that originate from intersubband transitions, known as *intersubband plasmons* [2,3], which show several similarities to surface plasmons of metallic nanostructures and have recently become of interest due to strong collective effects in the electromagnetic response [4]. We present a semiclassical theory of intersubband plasmons in quantum wells, based on nonlocal electrodynamics [5]. The theory is formulated in a very general way, and it can be applied to stratified geometries of any degree of complexity, including planar microcavities, where plasmon-polariton effects are predicted. Electrostatic coupling among different intersubband transitions gives rise to strongly radiative modes with subpicosecond radiative lifetimes. These modes are very promising for attaining a significant enhancement of light-matter interaction [6], up to the "ultrastrong coupling regime", where quantum and nonlinear phenomena, such as the dynamical Casimir effect, are expected to play a significant role.

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#### #P008 - Polydopamine: beyond its mussel-like features, towards bioelectronic applications.

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Multifunctional melanin-like polymers properties, i.e. broad band absorption in the UV-visible range, the hydration dependent hybrid protonic–electronic conduction and biocompatibility, inspired their implementation as active materials in bioelectronics application. Polydopamine represents an intriguing melanin-like polymer (black melanin-type) mainly know because of its filmability due to the high adhesive (mussel-like) feature. The attention was recently focused also on the polydopamine (pDA) optoelectronic properties, that are showing similarity with the eumelanin ones when embedded in metal–insulator-semiconductor (MIS) devices. pDA n-doping by in-air o-oxidation with aromatic amine resulted in the tuning of the MIS device functioning.

The incorporation within the pDA scaffold of pheomelanin units serving as photosensitizing component is an intriguing bio-inspired strategy for the enhancement of the pDA optical response. This strategy of implementing pheomelanin is based on the synthesis of 5-S-cysteinyldopamine product of metabolism, resembling the pheomelanin precursor 5-S-cysteinyldopa, and its copolymerization in variable percentage with dopamine p(DA/CDA). When embedded in p(DA/CDA) as the 'insulator' in MIS devices, the copolymer exhibits remarkable impedance properties closer to those of biological materials with a photocapacitive behavior at interesting

high frequency values of the AC voltage signal. The photoresponse is tunable via the feed ratio of DA and CDA monomers and found enhanced when increasing the CDA content.

#### #P009 - Early detection of ToMV and TyMV plant viruses via impedance spectroscopy characterization of textured silicon –based devices

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The early diagnosis of plant disease due to virus infection long before the disease is overt may represent a significant advance in the management of the virus effects by pharmacological therapy. A promising approach to boost the sensitivity of the virus detection can be developed through impedance spectroscopy by bio-electronic devices provided with textured silicon surfaces (TSi). TSi have been produced by plasma etching processes leading to the enhancement of the density of active sites for biomolecules detection due to the increase of the surface/volume area ratio (i.e. aspect ratio). The signal response of the virus/TSi hybrid devices can be furthermore improved by properly adjusting the wetting surface characteristics. The electrochemical interaction between viruses bearing differently charged residues with the textured surfaces can also enable the selectiveness between two different viruses. At best, with suitable morphological features of the surface texturing, intercalation of the virus in the structure is expected to result, thus allowing also fine selectivity with respect to the virus shapes.

In this framework, the present study is aiming to propose a plasma textured silicon surface based-device for a more sensitive detection of *Tomato mosaic virus*(ToMV) and *Turnip yellow mosaic virus*(TyMV). The electrical signal transduction across such a structure was evaluated via impedance spectroscopy technique. The results evidenced a high sensitivity to the virus species, a lowered concentration detection limit (about ng/ml), corresponding to the virus concentration development at the time when plants are asymptomatic.

A specific frequency (100 mHz) of the AC signal was found maximizing the device performance in terms of virus concentration detection. The results constituted a preliminary step for engineering portable devices embedding textured surfaces with the aim to "on site" evaluate plant health conditions.

#### #P010 - LIF study of N<sub>2</sub>(A) vibrational kinetics under nitrogen streamer conditions

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Non-thermal atmospheric-pressure plasma sources based on filamentary streamers generated in various discharge configurations (surface, volume, DBD, liquids) are emerging tools for various applications because they efficiently produce highly reactive species. The streamer creates a very thin channel containing various excited and reactive species during its propagation. Streamer discharges driven in nitrogen are characterized by substantial quantities of long-living (metastable) energy carriers (e.g. N<sub>2</sub>(A), N<sup>4</sup>(S), N<sub>2</sub>(X)) that are capable of affecting the physical chemistry of the discharge.

The evolution of individual v=0-10 vibrational levels of N<sub>2</sub>(A) metastable species produced by filamentary streamer discharge was investigated by the laser-induced fluorescence technique. Triggered single streamer filament was periodically produced in pure nitrogen at a pressure of 200 torr and metastable species were monitored during the streamer channel decay in the centre of the discharge gap. The observed dynamics of N<sub>2</sub>(A) vibrational levels follow two very different scenarios: while higher (v>6) vibronic levels decay exponentially in hundreds of nanoseconds, the populations of lower levels (v≤6) definitely increase, first reaching a local maximum on a microsecond timescale and then decreasing afterwards. Population maxima of N<sub>2</sub>(A<sup>3</sup>S<sub>u</sub><sup>+</sup>, v≤6) levels occur after the streamer onset with a certain delay, which decreases with increasing vibrational number. Interpretation of experimental observation based on a 0-D kinetic model of the post-discharge period takes into account the most important processes redistributing populations between the N<sub>2</sub>(A), N<sub>2</sub>(B) and N<sub>2</sub>(C) vibronic levels. The model reproduces experimental observations fairly well, including observed maxima delays occurring due to the collisional cascade, which transfers metastable species from higher even/odd vibrational levels towards v=0/v=1 terminal levels through the Δv=2 vibrational relaxation mechanism. A calibration procedure based on the rate of energy-pooling processes was used to determine absolute populations of the v=0 and 1 levels from LIF data, and the model results were utilized to place on an absolute scale all the higher (v>1) measured vibronic levels. Vibrational distributions obtained from calibrated LIF data at selected instants show a reasonable qualitative agreement with model predictions. Population maxima exceeding 2·10<sup>14</sup> cm<sup>-3</sup> were fixed for v=2 and 3 vibrational levels, while the lowest v=0 level reaches only 4-5·10<sup>13</sup> cm<sup>-3</sup>. Lastly, we show that the observed rate of the v=2 level decay is not compatible with published rate constants for the v=2->v=0 vibrational relaxation.

#### #P011 - Subnanosecond spectroscopy and imaging of low pressure N<sub>2</sub> streamer discharge

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A streamer is a frequent form of transient discharge which develops from an electron avalanche in an overvolted gap. The most important characteristics of such streamers are very high propagation velocity, a small streamer channel radius, and high density and mean energy of free electrons occurring in the streamer head. All these facts make laboratory streamers extremely difficult to observe with sufficient spatial (mm) and temporal (ps) resolutions.

Optical emission produced by streamers is determined by the spatial distribution of various species within the streamer channel that were excited to radiative states by streamer head electrons. Radial distributions produced by streamer electrons are strongly non-uniform because the maximum electric field of a propagating streamer occurs on the axis of the streamer and rate constants of the excitation, dissociation and ionization processes exponentially depend on the  $E/N$ . Radial non-uniformity of excited species have to be considered when using diagnostics with limited spatial and temporal resolutions or when comparing experimental results with numerical simulations.

In this contribution, evolution of optical emission produced by developing streamer filament in the DBD gap of 5mm was inspected by employing ultrafast ICCD diagnostic at 50torr in pure  $N_2$ . Due to the enhanced stability of the streamer discharge triggered by short nanoseconds high voltage pulse with sharp rise time of the order of few nanosecond and by employing technique of kinetic series with a variable width of ICCD intensifier gate, we have been able to achieve effective temporal resolution of tens of picoseconds. Such an enhanced temporal resolution allows resolving various phases of the streamer channel evolution, either through averaged ICCD images or ICCD spectra.

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### #P012 - Transition metals-graphene interaction: the role of the screened van der Waals energy

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The interaction of graphene with transition metals is of particular interest for practical applications, which include for instance the efficient production of high-quality graphene. The accurate theoretical description of transition metals-graphene interfaces, however, is a particularly challenging problem due to the complex interplay between van der Waals (vdW) and hybridization effects.

Here we apply the DFT/vdW-WF2s method [1], which allows to augment semi-local Density Functional Theory through the introduction of screened vdW interactions. Notably, we find that a reliable modeling of the van der Waals interaction should account for complex metal screening effects, that are due to the combined contributions of the p- and s-like \textit{quasi-free} electrons, and the more \textit{localized} d-states. The resulting geometry and energetic properties are in good agreement with experimental data and sophisticates theoretical calculations. Moreover, the Maximally Localized Wannier Functions underlying the DFT/vdW-WF2s method allow for an intuitive understanding of the complex binding mechanism. [1] P. L. Silvestrelli and A. Ambrosetti, Phys. Rev. B 87, 075401 (2013).

### #P013 - Statistical physics of nonlinear wave interaction

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The statistical physics approach to nonlinear optics consider the electromagnetic modes as classical spins interacting through a 4-body non-linear Hamiltonian, and the different emergent light emission regimes as different thermodynamic phases of the spin model. This approach has provided explanations for the Passive Mode-Locking transition [1] and it is supposed to describe a coherent wave regime with absence of long-range correlations in the Random Laser action [2, 3]. We have studied these relevant models, which are vector spin models with 4-body interactions on irregular topologies, beyond the Mean-Field approximation used in previous works [4]. We have found a rich and novel behavior, as the irrelevance of uncorrelated disorder (or dilution); the presence of a threshold beyond which the energy is non-equipartite; the absence of symmetry breaking in the presence of fluctuations; the vanishing of two-point correlators. These properties have consequences on real optical systems.

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**#P014 - Holographic Interferometry for the preservation of cultural heritage: characterization of hidden defects on paintings on wood by DSPI method**

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In the present study we tested the reliability and the performances of a compact Digital Speckle Pattern Interferometer for monitoring the whole body deformations of a painting on wood in out of laboratory conditions. Digital Speckle Pattern Interferometry (DSPI) is based on the traditional double-exposition holographic method, formerly utilizing special photographic plates and later electronic equipment. Nowadays DSPI is a well-established, non-contact and non-destructive testing technique, increasingly employed as a diagnostic tool in the field of cultural heritage. ESPI utilizes, in its basic implementation, a laser, a TV camera and a few optical components, providing non-contact, full field, sub-micrometric capacities. The object under examination is simply illuminated by a low intensity laser light and does not need any preparation. It is imaged onto the camera sensor where a reference laser beam is also superimposed. The output of a DSPI system consists of an interference fringes pattern (interferogram) overlaid onto the image of the object under examination. Fringes are produced numerically from two holograms of the object, recorded at different times, if some deformation occur, and can be regarded as a map of the surface displacement. Whole-body structural behavior as well as localized displacements can be evaluated at sub-micrometric scale. A large number of numerical methods have been developed for PC-based automated processing of DSPI interferograms, providing high spatial resolution and accurate, quantitative measurements. However, by utilizing former but still valid paradigms, the visual analysis of the shape and the number of such fringes can offer a simply interpretable evaluation of global deformations, as well as of hidden defects in restricted areas. Such a features can provide an intuitively user-friendly method for art conservators, not accustomed to high-tech or math based methods, in this way helping in disseminating the technique in that community. Despite DSPI has been applied in a number of cultural heritage applications, largely improving the traditional art diagnostics survey methods, it did not become a familiar tool in the art conservation field. Most of the studies, utilizing optical methods in artwork diagnostics, appear based on random, short term, interactions between research laboratory and cultural heritage conservation institutions.

**#P015 - Ce:YAG composites for white LED**

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Composites and luminescent polymers have been recently found to be potential candidates for the development of white LED, lasers and luminescent concentrators for solar cells. Due to its luminescence properties YAG doped with lanthanides ions is a good candidate as light emitting filler.

In a recent our work, the preparation of a polymeric nanocomposite containing Ce:YAG nanoparticles using in situ polymerization has been reported [1]. A good dispersion of Ce:YAG nanoparticles has been obtained maintaining them luminescence properties. In addition, an increase of thermal stability and stiffness of PMMA was observed [2]. Then, the preparation of Ce:YAG-PMMA composite has been performed by using the melt compounding method, which is not expensive, allows to obtain big quantitative of material, and limit the exposition at the carcinogenic monomer methyl-methacrylate used as starting precursor in the in situ polymerization [3]. In this work the preparation of Ce:YAG-PMMA and of Ce:YAG-PC composites by using the melt compounding method at several amount of Ce:YAG in the range 0.1-5 wt.%. is reported. Structure, morphology, thermal and mechanical properties of the composites were investigated. The optical properties of the obtained composites and of the composites combined with a blue LED were measured to investigate the effect of the Ce:YAG amount on the resulting emitted light in view of possible applications.

Results showed that the particles are homogenously dispersed in each polymer and that the thermal stability of the polymer and the optical properties depend on the filler quantity.

Acronym: YAG: yttrium aluminum garnet; PMMA: Polymethylmethacrylate; PC: polycarbonate.

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**#P016 - Neutron spectra for temperature and confinement diagnostics of imploded ICF plasma: models and 1D and 2D simulations**

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The spectrum of neutrons released by an inertially confined fusion (ICF) plasma provides valuable information on the emitting plasma [1] This includes, but is not limited to, ion temperature and confinement parameter  $\rho \cdot R$ .

For instance, a neutron-averaged ion temperature  $\langle T \rangle$  is obtained from the width of unscattered portion of neutron spectra. The confinement parameter is instead obtained from the ratio of the 14.5 MeV DT neutrons scattered in the 10-12 MeV range to the unscattered neutrons.

In case of a uniform source, at rest, the source spectrum is approximately Gaussian, with FWHM proportional to  $T^{1/2}$  [2] However, ICF imploded plasmas are space- and time-dependent, and plasma motion effects can also be important. Even neglecting scattering and secondary and tertiary neutrons, the spectrum is no more Gaussian, and this must be taken into account in the analysis of the emitting plasma.

As a first step in the development of a synthetic neutron diagnostics, we have written a neutron-source Monte Carlo package, taking into account thermal ion motion, bulk fluid motion, and elastic scattering. The package is coupled to the 2-D radiation-hydrodynamics code DUED [3].

We present neutron spectra obtained from i) 1-D simulations of exploding pushers; ii) simulations of targets with parameters analogous to the NIF record-yield high-adiabat implosions [4], iii) 1D simulations of igniting capsule implosions; iii) 2D simulations of shock-ignition targets. We discuss the effects of bulk motion (evident in exploding pushers and in targets with strongly distorted hot spots).

We also show how the spectrum FWHM is related to an appropriately weighted ion temperature, also including the effects of fluid motion.

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#### #P017 - PALM imaging of *Deinococcus radiodurans* with a mysterious fluorophore.

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PALM imaging of *Deinococcus radiodurans* with a mysterious fluorophore.

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Fluorescence nanoscopy based on PALM (PhotoActivated Localization Microscopy) or STORM (STochastic Optical Reconstruction Microscopy) usually relies on intensive work to achieve successful labeling of the target molecules to be imaged. In PALM, genetically encoded labeling is achieved using phototransformable fluorescent proteins that change their fluorescence state upon illumination, and sparse single-molecule activation is obtained through weak illumination of the sample with UV-violet light. In STORM, organic dyes are used through either antibody labeling or binding to specific peptide sequences or proteins fused to the target. Data collection then typically requires oxygen-free redox buffers that ensure efficient photoswitching of the dyes. In an effort to develop high-resolution microscopy of the strongly radioresistant bacterium *Deinococcus radiodurans*, we discovered that the membrane of this microorganism can be imaged at the nanoscale without any labeling procedure. This was achieved using standard buffers and a minimal PALM set up in which only a 561-nm laser is used for activation and readout. This finding originated from preliminary experiments aiming at evaluating the level of background fluorescence possibly produced by deinoxanthin, an orange-colored carotenoid molecule that scavenges reactive oxygen species and is responsible for the pink pigmentation of *D. radiodurans*. We collected PALM data on fixed control samples devoid of any engineered fluorescence labeling, and to our surprise, we observed pronounced and sparse single-molecule fluorescence localized at the bacterial membrane. The data allowed to reconstruct images of the *D. radiodurans* membrane at a resolution  $< 50$  nm. We looked at possible sources of fluorescent impurities that could be present in the medium and show pronounced affinity for the *D. radiodurans* membrane, effectively allowing a PAINT-like nanoscopy approach. However, although the amount of staining was not reproducible from colony to colony, efforts to eliminate it by changing or thoroughly cleaning all constituents of the sample (growth medium, PBS, water, fixative, cover-slides ...) were unsuccessful. Single-molecule fluorescence was also observed in live *D. radiodurans* cells and in a mutant strain in which the deinoxanthin synthetic pathway was impaired leading to an accumulation of the lycopene by-product. The molecule responsible for these observations thus remains to be identified. Its photophysical behavior measured at the single-molecule level will be presented in this poster.

#### #P018 - Properties and applications of plasma actuators based on Surface Dielectric Barrier Discharges

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Properties and applications of plasma actuators based on Surface Dielectric Barrier Discharges

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Surface Dielectric Barrier Discharges (SDBD) are atmospheric pressure cold plasma devices where microdischarges happen in a thin air layer just above an insulating material surface. Besides other uses, this feature makes these devices interesting for aerodynamics, being particularly suitable in order to energize the boundary layer of airflows surrounding objects, an application known as plasma actuator [1]. As a matter of fact, many experimental studies have proved that SDBDs can generate an induced airflow of several m/s. Here we present experimental results concerning the spatial structure of the induced flow, in particular when the discharge undergoes a transition to the filamentary regime.

On the other hand the plasma state produced in these devices consists of a high rate repetition of nearly independent discharge events happening in short times (a few tens of nanoseconds) and within a small spatial extension (a few hundreds of microns), i.e. microdischarges [2]. Here we present some results of an experimental campaign concerning the statistical properties of microdischarges which build up the SDBD. In particular we have studied single microdischarge current events, which have been measured with a fast current probe (100 MHz bandwidth) collected by a small portion of the electrode expressly sectioned [3]. Differences in the amplitude, duration and transported charge associated to the microdischarges have been measured in correspondence of various phases of the discharge events. This could be correlated with the induced velocity field, because the boundary layer flow is influenced by collisions between neutral air molecules and charged particles moving in the discharge region.

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#### #P019 - TiO<sub>2</sub> PHOTOCATALYTIC GLUCOSE CONVERSION TO H<sub>2</sub> AND HIGH VALUE CHEMICALS

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The conversion of biomass to chemicals has been the subject of intense research during the past decade. Different technologies are used to this aim as high temperature pyrolysis and gasification into syngas and bio-oils, conversion at supercritical conditions, biomass liquefaction, biological methods. The above methods suffer from some drawbacks such as harsh reaction conditions, high energy consumption, low selectivity. Heterogeneous photocatalysis can be considered a viable alternative since the process can be carried out under mild conditions of temperature and pressure. Glucose, which is a major component of biomass, can be used as a model compound for the sustainable production of high value chemicals. In this work it is reported the conversion of glucose in aqueous dispersion of various TiO<sub>2</sub> based photocatalysts. Aerobic and anaerobic conditions were used to study the distribution of the products both in the liquid (arabinose, gluconic acid, fructose and formic acid) and gas (H<sub>2</sub> and CO<sub>2</sub>) phases. Commercial and home prepared bare and Pt-supported TiO<sub>2</sub> samples were used as the photocatalysts. The Pt-TiO<sub>2</sub> samples have been tested under anaerobic conditions. The photoreactivity runs were carried out at room temperature in a 800 mL Pyrex cylindrical photoreactor irradiated in the UV region with a 125 W medium pressure Hg lamp. The initial aqueous glucose concentration was 1 mM. The identification and quantitative determination of its products were performed by HPLC whereas the CO<sub>2</sub> and H<sub>2</sub> evolution was followed by GC-TDC analyses. The distribution of the products was different in the presence of the various powders and the presence of Pt resulted essential for the anaerobic production of H<sub>2</sub> as no hydrogen was detected by using naked TiO<sub>2</sub> photocatalysts. The home prepared samples resulted more active than the commercial ones. The rutile polymorph was the most active sample both for glucose conversion and H<sub>2</sub> formation.

#### #P020 - Molecular mechanism of *Bacillus subtilis* GabR, a pyridoxal 5'-phosphate dependent transcriptional activator

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GabR is a transcriptional regulator belonging to the novel MocR/GabR family, characterized by a short N-terminal DNA-binding domain and a long C-terminal effector binding and/or oligomerization domain. The latter is structurally homologous to aminotransferases, a group of enzymes involved in amino acids metabolism that use pyridoxal 5'-phosphate (PLP) as a cofactor. In the presence of gamma-aminobutyrate (GABA), GabR activates transcription of the *gabT* and *gabD* genes, which encode two enzymes involved in GABA metabolism (GABA aminotransferase and succinate semialdehyde dehydrogenase, respectively).

The aim of the present study is to investigate the molecular mechanism of GabR gene regulation in *Bacillus subtilis*. In particular, we focused our attention on the GabR/DNA binding and on the role of PLP and GABA in this interaction. Spectroscopic analysis exploiting absorption and fluorescence emission properties of PLP indicate that GabR can react with cysteine, glycine and GABA with formation of covalent adducts. In the case of GABA and glycine an external aldimine is formed ( $K_D$ s of  $1.98 \pm 0.13$  mM and  $> 80$  mM, respectively). This result is somewhat surprising considering that in the case of GabR, and differently from PLP-enzymes, GABA is a regulatory cofactor and not the substrate, and GabR appears unable to complete the transamination reaction of the bound amino acid. Reaction with cysteine leads to the formation of a lanthionine external Schiff base which is released upon dialysis to give the GabR apo-form. No significant changes occur in the protein secondary structure upon PLP and GABA binding, as indicated by far-UV circular dichroism spectra. Since crystallographic studies reported that GabR is a head-to-tail domain-swap homodimer, we investigated the oligomerization state by gel electrophoresis and by atomic force microscopy (AFM). Particle volume analysis of GabR AFM images indicates a monomer-dimer equilibrium in the absence of DNA. Likewise, analysis of GabR/DNA complexes shows that GabR binds DNA as a dimer, regardless of the presence of PLP and GABA. Because these ligands have little effect on the DNA binding affinity of GabR, which falls in the tens of nanomolar range, the mechanism exploited to regulate transcription remains unclear.

Currently we are pursuing mutagenesis of both GabR and its target DNA sequence to identify the DNA sequence repeats involved in the specific binding of GabR and to assess the energetic contribution of the two protein domains to the protein-DNA interaction.

#### #P021 - Time-domain investigation of core-hole relaxation dynamics

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We investigated the ultrafast, sub-ps many-body relaxation dynamics in a metallic valence band following the creation of a high density of core-level holes by means of a time-domain pump/probe experiment, where core-holes were generated by a seeded FEL pulse (FERMI@Elettra), and the valence-band dynamics was probed by the reflectivity of an ultrashort near-IR pulse. The experiments were performed on aluminum films; Al has a simple electronic structure, consisting of a valence band, 2p core levels with around 73 eV binding energy, and deeper 2s and 1s states. Thus, at photon energies just in excess of the L<sub>2,3</sub> edge, the photoexcitation cross section is dominated by 2p-core-hole excitation, meaning that there exists a strongly preferential channel for soft-X-ray absorption in the material.

In order to selectively address the effect of a core-hole creation, the pump-FEL energy was swept across the 2p core-level absorption edge, while measuring the optical reflectivity with the probe beam, performing pump-probe reflectivity measurements with variable FEL energies both below and above the Al L<sub>2,3</sub> edge at 72.5 eV,  $\lambda \approx 17$  nm. Preliminary experiments performed on the EIS beamline@FERMI on 200-nm thick Al films (FEL fluence 25 mJ) show the feasibility of this complex experiment, and provide interesting clues about the FEL-induced excitation dynamics. In the short-delay regime, a major difference is seen in the visible-reflectivity change DR between above/below edge excitation. At larger delays, the  $\Delta R$  dynamics converge to a common trend, with a deep reflectivity decrease followed by a long-delay recovery, indicating possibly similar mechanisms of energy transfer from the electron gas to the lattice. In the very-short-delay regime, instead, the visible reflectivity behaviour is dominated by the effects of electronic excitation, particularly the way the hot-electron energy is redistributed in the valence band by electron-electron scattering, and then transferred to the lattice within the time scales of the electron-phonon coupling. In this respect, the simplicity of the Al electronic structure allows to isolate fewer electron energy-decay channels (e.g. Auger processes only for the Al 2p hole, valence-valence scattering for the excited electrons) simplifying the data analysis, although a full-fledged model will be required to interpret the data. A deep analysis of the short-delay dynamics might indeed grant access to interesting properties of nonequilibrium aluminium, like the electron-phonon coupling time, a case-study for more complex systems under analogous conditions.

#### #P022 - MARTINI Coarse-Grained Models of Polyethylene and Polypropylene

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The effect of micro and nanoplastics on living organisms is nowadays the object of intense research efforts from the toxicological point of view [1], but it is still largely unexplored at the molecular level. Here the main challenge is that the interaction between polymers and biological materials involves processes covering a wide range of time and length scales. Thus, fully atomistic simulations are often too cumbersome, and coarse grained (CG) models become very useful to capture many physical aspects that would remain unexplored because of computational time reasons.

We developed two coarse grained models of polyethylene and polypropylene, compatible with the MARTINI CG force field [2]. As a first step, we derived the CG bonded and non-bonded interactions, in a way to reproduce bonds, angles and dihedrals distributions in the melt obtained with a united atoms model. After that, our models were validated by comparison with experimental data and finer level calculations, in terms of structural and thermodynamic properties. The PE model is in excellent agreement with the available data, both in terms of density and radius of gyration in the melt. The PP model overestimates the melt density, while reproducing correctly the radius of gyration. As in its most common form PE is a highly branched polymer [3], we also developed and validated a PE model including branching units, reproducing the structural properties of Linear Low Density Polyethylene (LLDPE).

The behaviour of the polymer chains was tested also in different environments. The chains correctly collapse in water, and the scaling of the radius of gyration with the polymer size in a good solvent is in agreement with the theory. The conformational properties of the polymer chains in a PE/PP blend agree very well with the ones obtained with the atomistic model. In view of the application of our PE and PP models to the study of polymer-membrane interactions, we calculated the free energy profiles of dimers of PE and PP penetrating a POPC membrane. Our MARTINI models reproduce the atomistic free energy profiles very well, leading to the right water-membrane partitioning.

In summary, our CG PE and PP models perform well and are consistent with the MARTINI force field for lipids, paving the way to applications in the realm of both material sciences and biomedicine.

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#### **#P023 - FT-IR study of biopolymer-clay nanocomposites: effects of intercalation in montmorillonite on the properties of chitosan films**

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Chitosan-based nanocomposites at different sodium montmorillonite (MMT) loadings were prepared by solution casting. The MMT weight percent relative to chitosan was varied from 1 to 5% and the impact on the swelling and structural properties of chitosan film was investigated by X-ray diffraction and Fourier Transform infrared spectroscopy. In order to better discriminate the different functional groups involved in the interaction with the clay, the FTIR spectra were deconvoluted by a curve fitting procedure. The objective of the work was to correlate the physicochemical properties of the films to the nanostructures and the interactions occurring between the biopolymer and the clay. The XRD results evidenced that the intercalation of chitosan chains within the silicate galleries takes place to a different extent depending on the clay loading. The FTIR analysis, besides confirming intercalation, evidenced that the clay interacts with chitosan through hydrogen bonding involving primarily the amide groups. These interactions are responsible for the formation of a denser crosslink network that lowers the water sorption of the chitosan/MMT nanocomposites in comparison to the pure chitosan film.

#### **#P024 - Vents Pattern Analysis at Mount Etna volcano (Sicily)**

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Mt. Etna is the largest, as well as the most active volcano in the Mediterranean Sea. Volcanism started about 500 ky ago and the erupted magmas range from tholeiitic to alkaline affinity. An almost continuous summit activity characterizes the volcano; however, flank eruptions occur at an interval of years, mostly concentrated along the NE, S and W rift zones.

Volcanic hazard, in terms of map of future vent opening, will be explored by means of a spatial point pattern analysis of the known historical positions (154 flank vents) of the last 4.0 ka. The vents indicate that they cluster on a variety of spatial scales. Such clustering suggests that nonhomogeneous Poisson models should be used to forecast future vents distribution. That is spatial intensity (events per unit area) varies across the map region. For this reason, both spatial regularity (first-order feature, with density estimation) and clustering (second-order feature, with minimum distance separation among vents) in the Etna region at different distances are analysed. In particular, a Gaussian kernel technique (Connor & Connor, 2002) and the Ripley K-function (Ripley, 1976) are used to explore both features, respectively.

Some historical vents, which presently result covered, were extracted by the previous geological maps; other vents, mostly related to eruptions occurred before 1600 AD, were located after a reconstruction based on the portions of the lava flow fields still cropping out. The latter invoke an uncertainty, the measurement *error zone*, which is different from the spatial error, whose possible solution lies in the kernel density estimation, when the bandwidth is applied. Indeed, this bandwidth allows for the sampling error in the location (aleatory uncertainty), that describes what we would see if we could repeat the experiment by observing a different sample of flank vents. Therefore, both uncertainty sources have to be considered in a bandwidth that combines the sampling error and the measurement error (larger for poorly located vents).

Probabilities (retrieved after the density estimation application) have been calculated with the most significant values in line with the SSE sector of the volcano edifice, encompassing S rift as well as the upper slope of Valle del Bove, even though not negligible values were estimated along the NE and W rift areas.

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### #P025 - Automatized near-real-time short-term Probabilistic Volcanic Hazard Assessment of tephra dispersion before and during eruptions: BET\_VHst for Mt. Etna

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Tephra dispersal may heavily affect public health and critical infrastructures, such as airports, road networks, and electric power supply systems. Mainly for this reason and because there is an increase of number of explosive eruptions at Etna, three eruptive scenarios are daily run at the Istituto Nazionale di Geofisica e Vulcanologia, Osservatorio Etna, to forecast volcanic ash dispersal and fallout every 3 hours. However, although the results are very useful to give preliminary warnings the uncertainties are not treated. Probabilistic Volcanic Hazard Assessment (PVHA) represents the most complete scientific contribution for planning rational strategies aimed at managing and mitigating the risks posed by eruptive activity during volcanic crises and eruptions. Short-term PVHA (over time intervals in the order of hours to few days) must account for rapidly changing information coming from the monitoring system, as well as, updated wind forecasts, and they must be accomplished in near-real-time. In addition, while during unrest the primary goal is to forecast potential eruptions, during the eruptions it is also fundamental to correctly account for the real-time status of the eruption and of tephra dispersal, as well as its potential evolution in the short-term. In this work, we take into account both central and lateral eruptions that can generate short and long lasting activity respectively. For central eruptions we considered eruptive scenarios similar to the 12 January 2011, the 22 July 1998, the 5 January 1990 and 122 BC eruptions. For lateral eruptions the 2001 and 2002-03 eruptions were taken in consideration but we changed the location of the volcanic vent. Hundreds of simulations are carried out by a volcanic ash dispersal model and results are analyzed by the BET\_VHst model for Etna volcano. The model has its roots into present state deterministic procedure, and it deals with the large uncertainty that such procedures typically ignore, like uncertainty on the potential position of the vent and eruptive size, on the possible evolution of volcanological input during ongoing eruptions, as well as, on wind field. Uncertainty is treated by making use of Bayesian inference, alternative modeling procedures for tephra dispersal, and statistical mixing of long- and short-term analyses.

### #P026 - ZnO nanowires grown on bulk ZnO: elastic properties modification induced by deep-cryogenic treatment

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Deep-cryogenic treatment was performed on vertically aligned ZnO nanowires produced by metal organic chemical vapor deposition. The mechanical response of the nanowires was detected by nanoindentation tests. It was found that Young's modulus, the critical buckling stress and strain of individual nanowires is not significantly influenced by cryogenic exposure. Yet, the bulk base ZnO, from which the nanowires are grown, halved after a deep-cryogenic treatment.

**#P027 - Pressurization and depressurization phases inside the plumbing system of Mt. Etna volcano: evidence from a multiparametric approach**

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During 2013 Mt. Etna volcano experienced intense eruptive activity at the summit craters, foremost at the New Southeast Crater and to a minor degree at the Voragine and Bocca Nuova (BN), which took place in two cycles, February-April and September-December.

In this work, we mainly focus on the period between these cycles, applying a multiparametric approach. The period from the end of April to 5 September showed a gradual increase in the amplitude of long period (LP) events and volcanic tremor, a slight inflation testified by both tilt and GPS data, and a CO<sub>2</sub> flux increase. Such variations were interpreted as due to a gradual pressurization of the plumbing system, from the shallowest part, where LP and volcanic tremor are located, down to about 3-9 km b.s.l., pressure source depths obtained by both geodetic and CO<sub>2</sub> data.

On 5 September, at the same time as a large explosion at BN, we observed an instantaneous variation of the aforementioned signals (decrease in amplitude of LP events and volcanic tremor, slight deflation, and CO<sub>2</sub> flux decrease), and the activation of a new infrasonic source located at BN. In the light of it, the BN explosion probably caused the instantaneous end of the pressurization, and the opening of a new vent at BN, that has become a new steady source of infrasonic events. This apparently slight change in the plumbing system also led to the gradual resumption of activity at the New Southeast crater, culminating with the second lava fountain cycle of 2013.

**#P028 - Diagnostics for laser plasma generation using SiC detectors and Ion collectors**

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In the ambit of laser-matter interaction and in vacuum plasma generation, a fast diagnostic can be employed to detect the generated photons, electrons and ions streams. At low and high laser intensities a fast diagnostic can be applied by using SiC semiconductors and ion collectors connected in Time-Of-Flight (TOF) configuration. The advantages of such detectors are due to the SiC wide gap energy that permits to doesn't see the visible light plasma emitted, to the low leakage current of the semiconductor at room temperature, to the high radiation hardness and to the employment of a fast detection electronics using a high frequency storage oscilloscope. TOF spectra of SiC detectors and ion collectors performed at laser intensities from 10<sup>10</sup> W/cm<sup>2</sup> up to 10<sup>19</sup> W/cm<sup>2</sup>, obtained in different international laser facilities, will be presented and discussed.

**#P029 - AN ALGORITHM FOR AUTOMATIC ESTIMATION OF BACKGROUND SIGNAL OF RAMAN SPECTRA FROM BIOLOGICAL SAMPLES**

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Raman microspectroscopy is extensively used to investigate the composition and structure of a wide range of materials at microscopic level. In particular, it has been successfully applied to study the chemical content of biological samples (as biopolymers, cells and tissues) because it involves the detection of vibrational modes which are specific of the functional groups inside the sample, so constituting a sort of "fingerprint" of the analysed material [1]. In fact, the Raman spectra of biological samples are characterized by several peaks due to vibrational modes arising from a large variety of biomolecular functional groups.

However, so that the Raman microspectroscopy is able to provide reliable results, some obstacles have to be overcome. The main of these is the removal of spectral background signals, due to both intrinsic autofluorescence and stray light, which are usually a few orders of magnitude stronger than those related to Raman signal. Several computational methods have been proposed for rejecting the mentioned spurious signals and obtain the true Raman signals: among them, polynomial fitting is the most popular one, because of its simplicity. Nonetheless, such methods gives results which depend on the order of chosen polynomial function and often requires user selection of "non-Raman" locations on which to base the fit. So, several iterative methods, producing a background in an automated way, have been developed: the most widespread iterative method is the modified polynomial fitting method, which was originally proposed by Lieber and Mahadevan-Jansen [2] and successively improved by other authors [3].

In this work, a flexible polynomial background construction algorithm has been implemented in order to estimate the background of typical Raman spectra from cell samples. Such method is based on several subsequent steps: first of all, the boundaries of spectral regions containing Raman peaks bands are identified by approximating spectrum's derivative; then, many fitting are



performed by using polynomial functions of different orders for the different spectral regions; afterwards, for each spectral region the area underlying the polynomial fits are estimated and compared in order to exclude outliers polynomial functions; finally, for each spectral region a proper polynomial function is chosen for represent the background.

Substantially, our algorithm computes the background in a piecewise manner performing an efficient spline construction region by region. This method has been tested with synthetic and experimental spectra.

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### #P030 - Self-trapping and gradient-cooling of 2D polariton condensates

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Polariton condensation has been observed in many systems, ranging from standard 2D[1]

Polariton condensation has been observed in many systems, ranging from standard 2D[1] microcavities and 1D wires to confined pillars[2] and more recently using hybrid or organic dyes as active materials[3]. Although several aspects of the condensation dynamics and the formation of an extended coherent state of polaritons are well understood [4], the non-conventional out-of-equilibrium character of these hybrid states of light and matter regularly brings on stage unexpected phenomenology[5]. In particular, we have recently observed a surprising diffraction-limited self-localisation of the polariton condensate on the top of a potential hill, followed by ballistic expansion outside of the excitation region.

We explain these intriguing phenomena in terms of a self-trapping effect arising from the interplay of diffusion and thermalization, which leads to the formation of cold polariton drops at points of maximum potential energy. At higher excitation densities, the opposite situation occurs: a delocalized polariton condensate, thermalized at the lowest energy state of the dispersion, extends for hundreds of microns outside of the excitation spot. This condensate is constrained only by the slight differences in the sample potential minima and by the decreasing density of polaritons for larger distances from the excitation spot, and it is observed here for the first time thanks to the long lifetime of polaritons (high-Q sample used in these experiments). Its formation is the result of the interplay between energy relaxation from higher energies states and stimulated scattering towards the bottom of the dispersion, characteristic of bosonic particles. The phase transition is studied for increasing polariton densities by measuring the first order spatial coherence of the two dimensional polariton fluid.

These results show that much is left to explore in the high-density and ultrafast dynamics of polaritons, with a striking and unique phenomenology that could open new areas of research and applications not accessible to their atomic counterparts.

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### #P031 - Investigations on Laser Thermal Annealing on Germanium for High Dopant Activation

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Nowadays, there is a renewed interest in the use of Ge for advanced CMOS technology because of its superior electrical characteristics and lower temperature processes compared with Si, as well as its compatibility with the well-established silicon technology. Laser thermal annealing (LTA) process is gaining interest in the context of the 3D sequential integration where a locally confined thermal budget is needed for top FET to preserve the bottom FET from any degradation. Our aim is to investigate the effects of LTA on Ge based n-type ultra-shallow junctions to gain highly activated dopant concentrations.

We doped Ge with As or P by ion implantation with a dose of  $10^{15}$  atoms/cm<sup>2</sup> at 28 keV and 15 keV, respectively. Then we compared a LTA with a conventional thermal treatment in order to remove ion implantation damage and increase the dopant activation. We performed Raman spectroscopy, Transmission Electron Microscopy and Secondary Ion Mass Spectroscopy to study the disorder and the dopant diffusion after the LTA process. In detail, we studied the amorphous to crystalline phase transition as a function of the increasing LTA energy density. We found that using LTA, higher carrier concentration (above  $10^{20}$  cm<sup>-3</sup>) was achieved in n-type doped regions with respect the conventional thermal annealing.

These fundamental studies clarify the thermal effect of LTA on very thin (tens of nm) Ge films and could be considered for the fabrication of junctions in advanced 3D Ge-based devices.

### #P032 - Low temperature properties of unconventional ferromagnetic Josephson junctions

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Josephson junctions incorporating non-conventional barriers such as ferromagnetic insulators have been widely investigated in recent years [1,2]. These devices show a wide range of interesting properties such the low dissipation and spin polarization of the supercurrent, which makes them quite attractive for the realization of superconducting magnetic memories.

We have focused our attention on the study of the temperature dependence of the critical current and the characteristic voltage of ferromagnetic tunnel junctions down to low temperatures. Our preliminary results show different trends for junctions with different spin filter efficiencies. An anomalous behavior in presence of an external magnetic field is also observed. Results are discussed in the wide context of weak links to trace possible unconventional effects.

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### #P033 - High-throughput drug screening by Printing Biology

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*Printing biology* is our way to define a novel field employing material printing techniques generally used in plastic electronics to solve important issues of biology by miniaturized and high-throughput platforms. In this field, we already showed the possibility to use Dip Pen Lithography to fabricate single-cell biochips [1]. Also, we employed non-contact patterning methods such as inkjet printing methods to fabricate microarrays for drug screening at solid-liquid interfaces [2] or in picoliter-scale liquid droplets [3] so enabling high-throughput screening of chemical libraries onto disease-based targets. In this regard, printing methods would greatly reduce times and costs of standard drug screening campaigns which are commonly based on complex liquid handling robotics and are time and reagent consuming (micro-, nanoliter scale). In this work, we show a low-cost, general and miniaturized printing biology approach for drug screening, by combining Inkjet Printing and Dip Pen Lithography to develop the biochip. We show the possibility to precisely deliver femtoliter scale droplets of protein targets by Dip Pen Lithography by finely tuning the deposition parameters and ink formulation. Protein solutions are spiked with glycerol at 30 % v/v and are deposited at defined values of humidity (50 % -70 % R.H.). This permits to obtain microscale droplet arrays where picoliter volumes of drug candidates solutions are readily deposited by inkjet printing. In this way, it is possible to produce different drug targets concentration directly on-chip. Fluorescence confocal microscopy is here used to quantify drug-ligand interaction by means of standard intensity based imaging and fluctuation techniques that permit mapping concentration and important biophysical parameters including diffusion coefficients of fluorolabeled (or intrinsically fluorescent) ligands at nanomolar concentration. Outputs obtained on different systems by means of such a miniaturized approach are compared with the ones obtained on standard microliters volumes samples, confirming the ability of our *biochip printing* methodology to discriminate ligand-target interactions in different compounds. MiUR and the PRIN2012 program are acknowledged for fundings.

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#### #P034 - Electrochemical investigation of recovery mechanisms in dye sensitized solar cells. Evidence of lifetime improvement

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Electrochemical investigation of recovery mechanisms in dye sensitized solar cells. Evidence of lifetime improvement

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In this work we study the spontaneous recovery phenomenon present in solar cells sensitized with a Ruthenium complex based dye N719, which manifests with the increase over the time of the short circuit current ( $I_{sc}$ ) and the open circuit voltage ( $V_{oc}$ ) after the cell is illuminated, for durations of minutes up some days. We investigate the effects of temperature and type of components used in the electrolyte, based on iodide/iodine redox couple, using current-voltage measurements and electrochemical impedance spectroscopy (EIS) under dark and open-circuit conditions. The characteristic frequency peaks observed in the spectra, identified by Nernstian diffusion in the electrolyte, the diffusion and recombination of the photoinjected electrons in the  $TiO_2$  and the charge transfer at the platinum counter electrode, allow to determine the mechanism which causes the observed drifts. By impedance spectra modelling we determine the time evolution of the effective lifetime of the electrons in the  $TiO_2$ . The main result is that the life time of electrons in the oxide increases over time, confirming the recovery of the performances and that the phenomenon depends on the charge transport mechanism at the  $TiO_2$ -electrolyte interface. In particular the instability is induced by electron trapping by the defects present in the  $TiO_2$  created by ionic and molecular components present in the electrolyte that limit the recombination of electrons from  $TiO_2$  to the triiodide.

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#### #P035 - Characterization and development of a low cost system to evaluate beam quality in diagnostic radiology

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In our previous work a commercial silicon PIN-photodiode (Hamamatsu, mod. S2506-02) was tested and characterized as ionizing radiation detector for radiological applications in a wide range of configurations and effective energies: 17-19 keV (mammography) and 23-72 keV (conventional radiography and CT). In order to validate the dose response, the photodiode voltage output was compared to the readout of a Barracuda device (a semiconductor device used in clinical application), and Monte Carlo simulations were performed. Novel acquisition electronics was designed to amplify the PIN diode signal, based on a transresistive, non-polarized amplification current-to-voltage conversion stage using an OPA2340 operational amplifier. In order to investigate the reproducibility of devices from different production batches, two lots of 14 photodiodes each were irradiated simultaneously with X-rays and a small systematic difference (below 10%) was observed between the two batches: the difference is low but required different calibration factors. The angular sensitivity of the devices was investigated during CT and mammography acquisitions: the dose response showed a growing dependence on radiation angle of incidence moving toward lower effective energies. The sequential single slice CT acquisition, performed at slow rotational speed, showed a low angular dependence over the range of effective energies used. The photodiodes, inserted in a modular phantom, allowed the optimization of CT acquisition protocols in terms of diagnostic quality and dose received, which is especially important for pediatric subjects. The response uniformity was investigated in mammography over a large FOV: moving the devices along the axis of the acquisition plane showed a significant angular dependence over the range of low energies used, requiring different calibration factors. A low cost system was developed

with the characterized devices which can be used in every day beam quality measurements in terms of spatial uniformity, exposure rates and energies.

### #P036 - Experiments and computational investigations on HBx /Dleu2 lncRNA complexes: a possible “address code” to TRIM13 target.

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Long non coding RNAs (lncRNAs) are transcripts longer than 200 nt (1), recently recognized to exert a crucial role in epigenetics and in particular to modulate signalling pathways contributing to hepatocellular carcinoma progression (1,2). Assuming HBV-mediated carcinogenesis and HBV x protein oncogenic role, a possible molecular mechanism underlying lncRNAs expression and HBx has been recently investigated (3). Furthermore, Dleu2 contains within its genome the sequence of TRIM13 gene, implicated in autophagy (4,5). Comparative analysis has indicated that lncRNAs are evolutionarily conserved, and Dleu2/Trim13 was found to be conserved at the genomic level between human and mouse (6). A significant role of lncRNAs is the regulation of gene expression via a mechanism involving interaction with the epigenetic silencing complex Polycomb Repressive Complex 2 (PRC2).

In this work, we hypothesize that HBx can bind Dleu2, in turn linked to PRC2, so directing chromatin modifiers to specific genomic loci and particularly to TRIM13 promoter. Dleu2/HBx and Dleu2-Hbx/PRC2 proteins interaction has been investigated with bioinformatics tools (7-10) and RIP (RNA Immune Precipitation) experiments. The HBx structure was modelled by using I-TASSER, and the intrinsic disorder assessed by IUPred. Secondary and tertiary structure of 11 RNA exons were derived via DotKnot and RNAcomposer, respectively. Protein and exons models were then docked by using HEX and HADDOCK, to guarantee both an efficient sampling of mutual configurations and a more refined description of the interaction, including electrostatics. The different HBx-exon complexes were ranked; specific binding sites on HBx have been identified. A RIP experiment was also performed; the observation that, after HBx precipitation, Dleu2 is present in the sample, confirms a direct lncRNA Dleu2 /HBx interaction.

Docking of the complex Hbx-Dleu2, for some exons, with PRC2 proteins (EED, RBBP4, EZH2) reveals that the PRC2 proteins are competitors for the same binding site, while the HBx binding site is located in a different region of the same exon. We therefore propose a model (11) with three players, HBx-Dleu2-PRC2, in which HBx binding Dleu2/PRC2 disables the direct epigenetic silencing of specific regions of the genome where Dleu2 associates.

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### #P037 - X-ray nanodiffraction of free-standing Ge membranes

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Tensile-strained Ge is a promising candidate for a direct bandgap semiconductor which is compatible with existing Si integration technologies. However, the realization of tensile Ge within the SiGe-on-Si system requires approaches beyond simple two-dimensional heteroepitaxy [1,2].

Free-standing Ge membranes are a possible route towards this goal, since disconnection from the Si substrate allows much greater freedom to deform the structures with suitable stressors [3]. However, the lithographic processes required to create such

membranes themselves lead to variations in the properties of the material, which need to be characterized on the sub-micron scale. Ge membranes were fabricated by optical lithography and dry and wet selective anisotropic etching, in order to first define Ge mesas and then undercut the Si substrate from underneath.

Nanodiffraction experiments were performed using a nano-focused X-ray beam at the ID01 beamline of the European Synchrotron Radiation Facility in Grenoble. Fast-scanning X-ray nanodiffraction microscopy [4] was used in order to map the structural quality, strain state, and deformation of the Ge membranes. Nanodiffraction results were compared with finite-element method simulations, micro-Raman measurements, and large-area laboratory X-ray diffraction results.

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### #P038 - Graphene foams to tune the benefits of 2D materials for a 3D world

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Although 2D graphene has innumerable useful properties, in order to be exploited in many real world applications it must be manipulated into 3D structures. Ideally this should occur without any deterioration in electrical conductivity, to which chemically exfoliated graphene structures are prone. Instead graphene may be grown on templates of virtually any shape by Chemical Vapour Deposition (CVD), and in this way highly conductive, free-standing 3D graphene macrostructures called graphene foams (GF) were first produced from nickel foam templates in 2011 [1]. Since then there has been great interest in their use either alone or in composites with other materials in applications such as electrodes for supercapacitors [2] and Li-ion batteries [3], gas sensors [4] and adsorbents [5].

In this study, we grew GFs on metal foam templates using atmospheric pressure CVD. We were able to tune the number of graphene layers deposited and hence the robustness of the resulting foam by varying the type of template used (nickel or copper) and the flow rate of methane precursor. The resulting foams had a very low resistance, corresponding to excellent electrical conductivity. This is due to the fast transport channels created by the highly-branched, crystalline graphene network.

The pore sizes of the GFs grown by this approach were on the order of around 200  $\mu\text{m}$ . This is ideal for some applications (particularly biological), but many others would require a significant reduction of the pore size, for example for membranes or high density energy storage. To this end, we also synthesised 3D structures similar to GFs by CVD growth of graphene on Ni nanoparticles (<100 nm) annealed to form a network. The resulting GFs had a hierarchical structure, with both large (> 10  $\mu\text{m}$ ) and small (~1  $\mu\text{m}$ ) pores. These pores could eventually be controlled by compressing the Ni particles into pellets under varying pressures.

GFs are a highly promising way to bring the outstanding properties of 2D graphene to the 3D world. They have great potential for many different applications, as they have excellent electrical conductivity as well as mechanical properties. However, so far they have been largely limited by the size of the pores in commercially available metal foams. In this study, we have suggested an approach to overcome this limitation. Future work will focus on control of the pore sizes as well as introducing further interesting properties by exploiting the different growth mechanisms of graphene on different metal nanoparticle catalysts. [6]

- |     |                         |                  |     |        |         |
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### #P039 - Detection of topological phase transitions in the Josephson current-phase relation

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Experimental evidence of topological superconductivity has been based till now on probing the zero-bias conductance peak via tunneling spectroscopy. Here we propose an alternative and complementary tool to detect topological phase transition and the presence of Majorana edge states via the occurrence of discontinuities in the Josephson current-phase relation in a semiconductor-superconductor heterostructure in the presence of spin-orbit and magnetic field. Such discontinuities, which represent a sufficient condition for a transition to a non-trivial state, can be experimentally revealed by characteristic temperature and phase dependences of the current.

#### #P040 - The Transient Localization Scenario for Charge Transport in Crystalline Organic Materials.

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Understanding the microscopic mechanisms that govern charge transport in organic materials has been an open question for more than half a century. It is currently believed that the mobility in the best crystalline organic semiconductors is intrinsically limited by the presence of large thermal molecular motions, which are a direct consequence of the weak van der Waals inter-molecular bonds. These lead to an original regime of transport called transient localization, which shares features of both localized and itinerant electron systems. We concentrate on a commonly studied model which describes the interaction of the charge carriers with inter-molecular vibrations.

We describe in particular a relaxation time approximation which clarifies how the transient localization due to slow dynamical molecular motions relates to the Anderson localization realized for static disorder. Finally, we present a theoretical framework which identifies the optical conductivity as a fundamental experimental quantity to understand the charge transport mechanism. The relevance of the transient localization scenario to other classes of systems will be also briefly discussed.

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#### #P041 - EquilTheTA: a web-based tool for thermodynamics and transport properties of equilibrium plasmas

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EquilTheTA (EQUILibriumfor plasma THERmodynamicsand Transport Applications) is a web-based software which calculates chemical equilibrium product concentrations from any set of reactants and determines thermodynamic and transport properties for the product mixture in wide temperature and pressure ranges. The program calculates chemical equilibrium, thermodynamic

properties and transport coefficients starting from recent and accurate databases of atomic and molecular energy levels [1] and collision integrals [2].

Chemical equilibrium composition is a complex problem and many algorithms have been developed [3-5]. EquilTheTAIs based on a new approach [6,7], which consists in solving one equilibrium equation at a time. The algorithm is based on the idea of Villars [8] soon abandoned because the original method was not easily automatized. The reaction ordering is chosen determining, at each step, which reaction is farther from equilibrium, defining a reaction distance. The algorithm is very fast and stable, finding in very few steps the concentration of principal species and refining the solution of minority species in a second stage, this feature being adequate for fluid dynamic applications. A crucial aspect is the automatic determination of a shortcut reaction set that produces in a single step the same advancement resulting from hundreds of thousand steps with the original reaction set. In the calculations, Debye length and cut-off are consistently updated and virial corrections (up to third order) can be considered.

Transport coefficients are calculated by using high order approximations of the Chapman-Enskog method. The Eucken [9] approximation and the Butler-Brokaw [10] equation have been used for the calculation respectively of the internal thermal conductivity and of the reactive one.

Selected results for planetary atmospheres (Earth, Mars, Jupiter) are presented.

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#### #P042 - DFT investigation of polyalcohols reforming on palladium cluster

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Biomass conversion technologies have recently gained high industrial interest for the production of sustainable fuels and fine chemicals; starting feedstocks for these processes are generally complex mixtures of oxygenated compounds, ranging from lignans, carbohydrates and polyalcohols to carboxylic acids [1]. Framed within this scientific context the entire reforming mechanism of two well-known polyols, namely ethylene glycol (C<sub>2</sub>) and glycerol (C<sub>3</sub>), on a small Pd cluster was investigated by means of density functional theory. Among the large amount of reaction pathways that can be followed in the reforming of oxygenates, we discuss here only the route that brings to carbon monoxide and hydrogen as final products, since it is the most relevant in the biomass treatment.

It was found that the C-H bond cleavage, where the H atom transfers to the cluster, has an activation energy which is typical of such processes [2] and common to all the mechanism we will deal with. On the other hand, the rate determining step (rds) is the C-C bond breaking, with an activation barrier which exceeds the 160 kJ/mol. The same investigation applied to C<sub>3</sub> suggests that the mechanisms of the two studied polyols cross after the C-C reforming step, through a facile 1,2 hydrogen shift in a shared intermediate.

In order to obtain information on the reforming of heavier polyols, the rds was calculated for all the stereoisomers of C<sub>4</sub> (erythritol), C<sub>5</sub> (xylitol, arabitol and ribitol), C<sub>6</sub> (mannitol, sorbitol, galactitol and iditol), by including the influence of the position of the breaking C-C bond. Part of the reaction mechanism is in this case affected also by secondary interaction between hydroxiles and the palladium cluster.

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#### #P043 - Computational study of metal-free N-doped carbon networks as hydrogenation catalysts

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The future development and assessment of an industry more environmental friendly will include the use of metal-free catalysts. Most of the reported metal-free catalysts are homogeneous and often their recycle is difficult; therefore, develop and

investigate them is of interest both theoretical and experimental. Recently, N-doped nanotubes and graphene sheets, were synthesized [1,2], and it was demonstrated that the incorporation, within these carbon structures, of nitrogen atoms causes a greater electron mobility and introduces more active sites for catalytic reactions. This investigation is aimed at elucidating the main features of the hydrogen fragmentation over these carbon frameworks. Several models and different theoretical approaches were employed in this investigation to characterize the structure and properties of nitrogen pyridinic moieties framed within a carbon network, commonly classified as pyridinic defects. Two different kinds of pyridinic defects configurations within a carbonaceous environment were studied. The influence of the size of the  $\pi$ -system and of the curvature on the ergonicity associated to the  $H_2$  bond cleavage were analyzed. It was found that increasing the number of the benzene rings surrounding the defect the ergonicity of the reaction increases whereas the curvature of the carbon network scarcely affects this quantity.

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#### #P044 - UV irradiation of Methanol ice: role of the substrate

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Complex organic molecules have been detected in a lot of different astrophysical environments. Both very simple molecules like water ( $H_2O$ ), carbon monoxide (CO), carbon dioxide ( $CO_2$ ) and other more complex, e.g. methanol ( $CH_3OH$ ), have been found in molecular clouds and hot cores (Wooden et al. 2004). However, the origin of these molecules is still controversial and many kinds of reaction pathways have been taken into account. Gas-phase reactions are not sufficient, given the low densities of the astrophysical environments. Solid-phase (ice) reactions are much more probable and can be induced by radiation. Radiation leads to the destruction of molecules, forming fragments and radicals, which in turn can react and form new, more complex, molecules. In the last decades a lot of experiments have been carried out in order to evaluate how radiation affects the ice chemical complexity. Interstellar ice analogues have been irradiated by Ultraviolet (UV) radiation and X-rays and the ice evolution has been studied. The results have given insights on the ice chemical evolution and contributed to the interpretation of the astrophysical environments. We used the Life Irradiation Facility for Exochemistry (LIFE) to irradiate a  $CH_3OH$  ice with an UV source that provides Ly- $\alpha$  and hydrogen molecular emission, in order to study the chemical evolution as a function of the ice thickness and the substrate composition.

#### #P045 - A new structural model of the human $\alpha 7$ nicotinic receptor in an open conformation.

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Nicotinic acetylcholine receptors (nAChRs) are ligand-gated ion channels that regulate chemical transmission at the neuromuscular junction [1]. Structural information is available at low resolution from an eukaryotic receptor, and at high resolution from two prokaryotic and an eukaryotic GluCl channel; and from a water-soluble homologue of the LBD of nAChRs, the pentameric acetylcholine binding protein, which has been co-crystallized with a number of agonists and antagonists [2,3].

Structures of human channels however are still lacking. Homology modeling and Molecular Dynamics (MD) simulations are valuable tools to predict structures of unknown proteins, however, for the case of human nAChRs, they have been unsuccessful in providing a stable open structure so far. On one side the homology with prokaryotic species is too low, while on the other the open eukaryotic GluCl proved itself unstable in several MD studies and collapsed to a dehydrated, non-conductive conformation, even when bound to an agonist.

In this work, we provide an all-atom structural model of the open human  $\alpha 7$  nAChR in complex with the agonist epibatidine. To prevent channel closure we employ a restraint that keeps the transmembrane pore open, and obtain in this way a stable, hydrated conformation. To further validate this conformation, we run four long, unbiased simulations starting from configurations chosen at random along the restrained trajectory. The channel remains stable and hydrated over the whole runs; this allows to assess the stability of the open conformation over a cumulative time of  $1\mu s$ , 800 ns of which are of unbiased simulation. Analysis of pore hydration and size, as well as ions distribution, interface between domains, protein hydrogen bonds network, and epibatidine conformations at the binding sites support the picture of a fully active structure both in the extracellular and transmembrane regions.



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#### #P046 - Proteins in saccharides matrices: biochemical and biophysical aspects

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Embedding biomolecules in saccharide matrices leads to a series of peculiar properties that are relevant from the point of view of both biochemistry and biophysics, and have important implications on related fields such as food industry, pharmaceuticals, and medicine. In this poster we present results from a combination of experimental (FTIR, SAXS, DSC, Light Scattering) and simulative (MD) techniques on solutions or glassy matrices of oligo- and disaccharides at different water content, rigidity and temperatures, both in the presence and in the absence of proteins. The perspective is to set up a connection between the biophysical approach, which is generally "protein-centric", and the pharmaceutical/applicative approach, which is traditionally "stabilization-procedure centric". The attention is addressed in particular to the modulation of systems dynamics, to its hydration, temperature, and composition dependence, and to the molecular origin of the trehalose peculiarity.

#### #P047 - Nanoring as logic gate and memory mass device

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We study the application of one nanoring driven by a laser field in different states of polarization in logic circuits. In particular we show that assigning boolean values to different state of the incident

laser field and to the emitted signals, we can create logic gates such as OR, XOR and AND. We also show the possibility to make logic circuits such as half-adder and full-adder using one and two nanoring respectively. Using two nanorings we made the Toffoli gate. Finally we use the final angular momentum acquired by the electron to store information and hence show the possibility to use an array of nanorings as a mass memory device.

#### #P048 - Influence of the nanometer scale ring structure on the vibrational and relaxational dynamics of glasses

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Although glasses have been largely used for a wide variety of technological applications, much of their underlying structure and dynamical properties remain puzzling. We present a detailed investigation of the intermediate range structure of a series of alkaline borate glasses carried out by performing neutron diffraction measurements. We propose that the First Sharp Diffraction Peak of glasses arises from the periodicity of the boundaries of voids in a random network and put forward a model which explains its compositional and pressure dependence. In this model the planar section of a void is a n-membered ring of all-side vertex sharing basic structural units. Furthermore, we establish a correlation between the low frequency vibrational dynamics, the structural relaxation processes and the presence of voids on the nanometer length scale in several ring structured systems.

#### #P049 - Highly flexible, conductive and transparent ZnO:Al/Ag/ZnO:Al multilayer electrode

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The increasing interest in flexible devices, such as touch screens, solar cells and wearable electronics, has led to a great need for mechanically robust transparent electrodes. Indium tin oxide (ITO) and aluminum-doped zinc oxide (AZO) are well known transparent conductive oxides (TCO) and their reliability on flexible substrates have thus received attention by many researchers. However, for flexible applications the TCO film should to be as thin as possible without compromising its conductivity.

We have already reported how the addition of 10 nm Ag mid-layer to a AZO film is highly beneficial, allowing to strongly reduce the TCO thickness to about 100 nm, by maintaining, at the same time, a high optical transparency and an excellent conductivity [1]. However, thus far, there are very few studies that investigate the bending behavior of TCO/metal/TCO structures. We here report the effect of bending on the electrical and optical degradation of AZO/Ag/AZO multilayers (50nm/10nm/50nm), and for comparison of two AZO single layers (one with the same thickness of 110nm and one seven times thicker), deposited at room-temperature on flexible polyethylene naphthalate (PEN) plastic substrates. The electrical stability, optical transmittance and film damage (crack size and density) of samples under bending cycles were evaluated by I-V (percentage change in the electrical resistance), UV-Vis spectroscopy and scanning electron microscopy. Bend experiments were performed varying the radius and number of cycles. We observe excellent electrical stability and high mechanical flexibility in the AZO/Ag/AZO sample, whereas this is not the case for the single AZO films. The experimental results and the numerical simulations provide clear evidences of the key role played by the ductile Ag interlayer that provides improved robustness under mechanical strain.

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#### #P050 - Quantum measurement process by the parametric representation

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We present a description of the quantum measurement process based on the parametric representation with environmental coherent states. Such representation is specifically suitable for studying open quantum systems whose environment has to be considered through the quantum-to-classical cross-over. Focusing upon projective measures, we consider the standard (von Neumann) model to describe the pre-measurement process and the dynamical generation of entanglement between the system and the environment, and briefly discuss the role played by decoherence: In order to illustrate the formalism, the two paradigmatic models of spin and bosonic environments are considered. Exploiting the connection between large-N quantum theories and the classical limit of related ones, we finally manage to push our description beyond the re-measurement step, showing that the outcome production follows from a global-symmetry breaking, entailing the observed system's state reduction; the probabilistic character of quantum measures appears thus related to the macroscopic character of the measuring apparatus.

#### #P051 - variation of SO<sub>2</sub> explosive degassing prior to and after the August 2014 effusive eruption of Stromboli volcano (Eolian islands, Italy)

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Here we report a novel dataset on the SO<sub>2</sub> masses released by strombolian explosions prior to and after the August 2014 eruption of Stromboli volcano. These data were acquired with two fully autonomous permanent SO<sub>2</sub> camera devices installed at two sites located at 0.5 km (Rocchette) and 1.75 km (Sciaradelfuocorim) from the crater terrace. A two dimensional integration was used here to calculate the SO<sub>2</sub> mass from individual explosive bursts at three different crateric areas. The analysis has been carried out with a stand-alone user-friendly program called "Vulcamera". The strombolian eruptions have shown a decrease in SO<sub>2</sub> contents during the sequence of lava overflows in June and an increase (up to 150-200 kg of SO<sub>2</sub>) weeks prior to the eruption. After the onset of the effusive eruption the strombolian activity dropped as well as the released SO<sub>2</sub> masses that slowly returned to background levels after months. We interpreted this variation as a process of gas-magma drainage, due to the lava overflow/effusion, that reduces the amount of gas available to create the gas slug in the shallow conduits. Our observations offer new insights for the understanding of degassing dynamics within shallow conduit systems of Stromboli volcano.

#### #P052 - Photoneutron equivalent dose measurements around high energy LINACs

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This paper presents in-air and in-phantom measurements of photoneutron equivalent doses in external radiotherapy. These data are necessary to assess organ-averaged equivalent doses to derive the risk of secondary cancer development, associated with non-target organ exposures. The in-phantom dose measurements were carried out in a BOMAB-like water-filled phantom, by means of superheated emulsions. Dose data were acquired in a three-dimensional matrix of reproducible measurement points, which are spaced according to detectors size. Various treatment schemes, including clinical protocols for the treatment of a prostate tumor were considered and compared, by measuring the doses delivered to the planning target volume (PTV) and to peripheral

radiosensitive regions (i.e. colon- rectum and bladder). Radiation qualities of 6, 12, 15, 18 and 20 MV were used; all of these are capable of producing photoneutrons. Data from this work span most of the X-ray beam energies and prostate treatment modalities used in the current clinical practice. These data permit the assessment of doses absorbed by a radiotherapy patient either at the treatment volume or at out-of-field organs. It was in particular found that photon acceleration energies as low as 6 MV are able to produce a non-negligible photoneutron component, which causes an undue dose to the patient of the order of tens microsievert per unit photon dose delivered at the target volume.

#### #P053 - Synthesis of multiphase titania nanoparticles during laser ablation of titanium in water

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Laser ablation of solid targets in liquid environments has been established as a simple, straightforward and environmentally friendly method for the synthesis of nanoparticles with desired properties [1]. During under-liquid ablation a large number of phenomena, far from the equilibrium condition, can be responsible for the formation of a variety of exotic compounds, shapes and phases at the nanoscale level. It has been reported that the ablation of titanium target in pure water gives titania nanoparticles in suspension. These particles possess properties (size, defects states and stoichiometry) matching the requirements for the achievement of active layers in hybrid solar cells[2] or to serve in several environmental protective tasks such as active photocatalytic dye removal or direct and ultrafast H<sub>2</sub>O<sub>2</sub> assay[3]. While nanosecond laser ablation of Ti targets in liquid water leads to the synthesis of multiphase TiO<sub>2</sub> (anatase, rutile, brookite), a major challenge is actually to go deeper into the nanoparticle formation mechanisms and to establish experimental strategies in order to control and finely tune the characteristic of the nanoparticles produced.

This work shows that the ablation parameters, such as the laser fluence, the ablation time, the radiation wavelength are interconnected with the crystalline phase of the nanoparticles produced as well as their shape and size. For instance short ablation times (few J/cm<sup>2</sup>) and low infrared laser fluences give mostly particles as small as 10-30 nm in the rutile phase, while an overall increase of the anatase phase quantity, coupled with the increase of the particle size up to the micro-size range (100-400 nm) is observed when these conditions are changed. Traces of brookite in some experimental conditions are detected. Direct experimental observations through electron microscopy and X-ray diffraction are supported by Raman mapping and Luminescence data.

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#### #P054 - The table top high frequency lasing device

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Atomic and molecular systems, subjected to intense laser pulse, emit typical High-Order Armonic Generation (HHG) spectra. This work aims to investigate the possibility to obtain a laser device by HHG. At this end, we analyzed the emission spectra by a molecular ion driven by a linearly polarized laser field. The temporal behaviour is obtained using the Morlet wavelets transform of emission. The results show that, after filtration of the electromagnetic radiation emitted, it is possible to select a frequency which seems to have almost constant intensity and phase. This characteristic makes possible that HHG from a molecule can be used as high frequency laser fields.

#### #P055 - Risk assessment for natural gas emissions in the Hellenic territory

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Quantification of gaseous emissions in geological systems is an important achievement as it is a major source of greenhouse gas to the atmospheric budget. There are two different categories of geological environments: the first includes emissions of the predominant carbon dioxide (CO<sub>2</sub>), while the second includes emissions of the predominant methane (CH<sub>4</sub>).

The geodynamic setting of the Hellenic territory is very complex and derives from a long and complicated geological history. It is strongly characterized by intense seismic activity and enhanced geothermal gradient. This activity, with the contribution of an active volcanic arc, favours the existence of many cold and thermal gas manifestations. Geogenic sources release huge amounts of gases, which, apart from having important influences on the global climate, could also have a strong impact on human health.

A preliminary estimation of the gas hazard has been made for the last 20 years considering the whole population of Greece. In this period at least 2 fatal episodes with a total of 3 victims could be certainly attributed to CO<sub>2</sub>. This would give a risk of  $1.3 \cdot 10^{-8}$  fatality per annum. Such value, probably underestimated, is much lower than most other natural or anthropogenic risks. Nevertheless this risk, being unevenly distributed along the whole territory, should not be overlooked especially in areas with high density of gas manifestations and high soil gas fluxes.

Gas output estimations are at present available only for a few of the gas manifestations. This catalogue will be basis for a preliminary estimation of the total gas output of Greece.

#### #P056 - Morphological and electrochemical characterization of flame-made TiO<sub>2</sub> nanoparticle coatings for aluminum surfaces prepared by direct thermophoretic deposition

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In this work, a one-step method for the coating of aluminum surfaces with titania nanoparticles is presented. Narrowly sized, ultra-fine TiO<sub>2</sub> nanoparticles were synthesized by Flame Aerosol Synthesis and directly deposited by thermophoresis onto cylindrical samples of aluminum AA2024. Submicron coatings of different thickness and porosity can be obtained by varying the total deposition time. Two flame synthesis conditions were adopted in order to study the effect of particle size and phase composition on the properties of titania coating. Fuel-lean synthesis condition was used to produce 3.5 nm diameter pure anatase nanoparticles, while a mixture of rutile and anatase nanoparticle of 30 nm in diameter, rutile being the predominant phase, was synthesized in fuel-rich non-sooting condition. Scanning Electron Microscopy were used to characterize morphology and porosity of titania films, while coatings thickness were derived from Confocal Microscopy measurements. Electrochemical analysis was performed by means of Electrochemical Impedance Spectroscopy, with the aim to characterize the capacitive behavior of coatings through the analysis of impedance phase angle and modulus, which is an index of its capability to protect the sample.

#### #P057 - Modelling spatio-temporal dynamics of phytoplankton distributions in Mediterranean Sea

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Recently, theoretical studies were able to reproduce real vertical distributions of phytoplankton biomass in marine ecosystems. However, seasonal variations are not usually included in models which analyze the spatio-temporal dynamics of phytoplankton distributions in real aquatic systems. On the other hand, random and deterministic changes in environmental variables are responsible for significative consequences throughout the food chain, in particular in fish species, whose abundances are strictly connected with seasonal changes in the chlorophyll concentration, a marker of phytoplankton species. Here we present a one-dimensional stochastic reaction-diffusion-taxis model which allows to reproduce the spatio-temporal dynamics of five picophytoplankton populations distributed along a water column in a marine ecosystem. The model consists of stochastic differential equations, which include the effects of random and deterministic (seasonal) variations of environmental variables. The equations of the model are solved by numerical integration for different values of the noise intensity, obtaining for each picophytoplankton population the vertical distribution of biomass concentration as a function of the time. The numerical results, expressed in cell/m<sup>3</sup>, are converted in total concentration of *chlorophyll a* (*chl a*) and *divinil-chlorophyll a* (*Dvchl a*), obtaining chlorophyll distributions along the water column. These theoretical profiles are compared with experimental data for the chlorophyll concentration collected in a site of the Tyrrhenian Sea during four different periods of the year. In particular, for suitable values of the noise intensity a good agreement (checked by  $\chi^2$  goodness-of-fit test) between theoretical and experimental chlorophyll distributions is obtained for all periods (seasons) investigated. Our findings confirm that the phytoplankton abundance is strongly dependent on the oscillations of light intensity and depth of thermocline, deterministic (seasonal) spatio-temporal behaviour of the vertical turbulent diffusivity, and random fluctuations of environmental variables. These results could be useful to analyze phytoplankton dynamics in different marine ecosystems and predict future changes in phytoplankton abundance, contributing to devise strategies able to prevent the reduction of phytoplankton biomass and consequent decrease of fish species.

**#P058 -  $\gamma$  and X ray irradiation effects on H<sub>2</sub> unloaded and loaded P doped optical fiber**

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P doped optical fibers are employed for the production of optical amplifiers and laser [1]. In silica the P is mainly inserted in O=PO<sub>3</sub> tetrahedra, in which the P forms a P=O linkage [2]. P related radiation induced defects are responsible for optical absorptions (OA) that modify the fibers transmitting features. Griscom identified two paramagnetic phosphorous oxygen hole centers (POHC) named stable and metastable. The first is considered the origin of OA bands at 2.2, 2.5 and 5.3 eV, while the other is considered responsible for an OA band at 3.1 eV [3]. In P doped fibers H<sub>2</sub> loading was employed to produce fiber bragg grating [4], these materials feature lower radiation induced OA in the visible range [5] and a reduction of the induced POHC [6]. In this work we studied irradiated P doped fibers by electron paramagnetic resonance, Raman and confocal luminescence microscopy spectra to deepen the understanding of the radiation effects. The data indicate that stable and metastable POHC are induced. Under  $\gamma$  irradiation from 1 to 7.8 MGy their concentrations appear independent from the dose. The Raman spectra indicate that the radiation does not modify the matrix of the doped regions. Finally, under the X-ray irradiation we proved that the H<sub>2</sub> loading decreases the amount of the induced POHC even if the irradiation is performed several days after the loading, this result being relevant for their concrete application.

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**#P059 - Ionic and covalent functionalization of a layered perovskite with organic moieties: towards hybrid proton conductors**

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The design of innovative proton conductors for intermediate-temperature fuel cells, closing the gap between PEMFC and SOFC, is a forefront research theme in materials chemistry. [1] The HLaNb<sub>2</sub>O<sub>7</sub> layered perovskite (HLN) can be functionalized between the perovskite sheets to yield inorganic-organic hybrids: the intercalation of amines, alcohols, carboxylic or phosphonic acids, and their covalent binding to the sheets has been demonstrated recently. [2-3]

We present results on the ionic intercalation and covalent bonding of different organic molecules to HLN in order to develop hybrid proton conductors for use in intermediate temperature fuel cells: XRD, TGA, IR, and <sup>1</sup>H, <sup>13</sup>C and <sup>29</sup>Si NMR, are used to elucidate the intercalation process, together with ab initio periodic DFT [4].

Amines (histamine, octylamine, decylamine) and imidazole enter the interlayer space as cations, interacting ionically with the oxide sheets; mercaptopropyltrimethoxysilane and decanol bind covalently to the oxide layers. The use of sonication is shown to improve dramatically the reaction yield and to reduce the duration of syntheses. [5]

The ionic conductivity of hybrid materials is evaluated up to 300 °C.

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**#P060 - Laser induced fluorescence diagnostics of atmospheric pressure plasma jets**

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Critical requirements for the detection of transient species in atmospheric pressure (ATP) discharges are sensitivity, time and space resolution. This is particularly true in plasma jets flowing towards a humid target, that are typical devices in plasma medicine applications. The gas mixture composition and the physics of the discharge strongly depend on the presence of the target, and local discharge conditions change in a sub-mm space scale. In addition the voltage source excitation is often pulsed. Laser Induced Fluorescence (LIF) is the technique that satisfies these needs. LIF is based upon the absorption of laser photons by a molecular lower state, the state to be probed, and on the observation of light (fluorescence) emitted by an upper state. In single-photon LIF the upper and lower states are linked by a dipole-allowed ro-vibronic transition which the laser is tuned to. The observable is then a complex function of both the absorption rate and the collision and radiative properties of the upper state.

The spatial resolution of LIF is determined by the geometry of the experiment. The optical axis of the fluorescence detection arrangement is usually perpendicular to the laser beam, and the relevant collection optics contains a slit or an iris imaged onto the sampled region by a lens assembly. The sampled volume is the intersection of the slit/iris image with the laser beam. It can typically be a cylinder with diameter and height of the order of 0.1 mm with a focused laser beam. The temporal resolution is achieved by pulsed tunable lasers, and is determined by the pulse duration, that is of the order of 10 ns. Both time and space resolutions of LIF are suitable for a detailed characterization of ATP plasma jets.

In this paper we give a general description of the LIF technique by way of OH absolute measurements two plasma jet systems, namely a "plasma gun" [1] and a RF plasma jet [2]. We address in detail: the modelling of the LIF measurement, taking into account collisional processes and the spatial non-uniformity of the laser beam; saturation characteristics; absolute calibration; rotational temperature measurements.

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### #P061 - Plasma actuation to enhance the flame stabilization in a non-premixed lean microburner

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The demand of micro-devices is growing up especially for application such as micro-robots and micro-airplanes. The bottleneck for the development of such devices is the low energy density of the most common batteries. Building efficient micro-combustors has proven difficult. The major challenges are connected with the reduced dimensions that produce a high ratio between surface and volume of the device. Both the fluidodynamics and the heat loss are influenced by this ratio. Efforts in R&D are necessary to produce micro systems on a large scale. A promising burner configuration is the plasma assisted combustor. There are numerous works about the application of plasma for flame control, generally applied to macroscale combustor devices. Interesting works are those of Kim et al. [1], Cha et al. [2] and Pilla et al. [3] where a coaxial combustor was chosen for the experiments, with different plasma actuator technology: a dielectric barrier discharge (DBD) in [1], a glow type and the actuation affecting both reactants in [2] and a nanosecond repetitively pulsed plasma in [3]. Based on the aforementioned considerations, in the present work a micro-burner design with a high-frequency DBD discharge was employed to investigate the influence of plasma actuation to stabilize a lean non-premixed methane/air flame at atmospheric pressure and under different fuel/air ratios. We found that the plasma actuation enhances the flame stability of a micro-burner especially at lean combustion conditions. The plasma action resulted evident in an increase of the flashback and the blowout limits. The fuel/air ratio range in which flame is guaranteed is evidently enlarged by the plasma actuation. Furthermore a change of the flame shape was recorded using visual observations due to the increase of the flame propagation speed. The enlargement of the stability region permits to use ultra-lean mixtures and to emit less pollutants into the atmosphere while maintaining a stable flame. The plasma assisted combustion is shown to be a promising way to answer to the energetic needs of microscale devices.

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**#P062 - EFFECT OF MIXED DISORDER ON MINIBAND STRUCTURE AND RESONANCE ENERGY OF GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As SUPERLATTICES**

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Theoretical analysis of mixed disorder (association between topological and structural disorder) on resonance energy and miniband structure formation for rectangular GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As superlattices is presented in this study. The Airy functions model based on the transfer-matrix technique with the assumption of the effective mass approximation and using Bastard's boundary conditions are applied to Schrodinger's equation for an asymmetric potential. A detailed analysis of the resonance energy and miniband formation is given.

The transmission spectra reveal the appearance of a miniband structure with a concomitant disappearance of the localized states. The possibility of the creation of resonant states, with a good control of the energy differences is pointed out. Also the high bias voltage led to the emergence of a phase transition from the metallic state to the insulating.

The results show that for structures with short range correlation and stronger disorder, the electronic states of the system are delocalized since the localization length is greater than the system size. The quantum states in the well play a key role in the transmission.

Compared to other types of disorder structures already studied by the authors [1-2], we have shown in this study that the mixed disorder which is a combination between topological and structural disorder, gives the miniband that resists well to low applied bias voltages.

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**#P063 - The self-diffusion in the systems with geometric constraints**

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The magnetic fluids are the systems consisting of single-domain magnetic particles suspended in a carrier liquid. They have a wide area of applications, in particular, in medicine. The diffusion properties reply for a correct application of magnetic fluids in medicine. There were several works dealing with the diffusion study [1 – 4].

We consider the quasi-two-dimensional case of magnetic fluids. We have monodisperse (with one type of magnetic particles) and bidisperse (with two types of nanoparticles) systems. In our theory we suppose that the main structures are chain aggregates and rings. So the monodisperse ferrofluids contain one type of chains and one type of rings. A microstructure of a bidisperse magnetic fluid is more complex, and we consider 19 classes of chains and also rings consisting of large particles only.

We use Density Functional Theory to calculate the concentrations for chains and rings. After that we can obtain the mobility and self-diffusion coefficients for different structures. We find how the self-diffusion coefficient depends on magnetic dipole-dipole interaction parameters of small and large particles and small and large particles area fractions.

Also we perform the molecular dynamics simulations using ESPResSo [5] to calculate the self-diffusion coefficients. We consider two types of systems: magnetic systems with magnetic dipolar particles and "nonmagnetic" systems with soft spheres. We can obtain the self-diffusion coefficients for both magnetic and nonmagnetic systems. Then we divide the coefficient for magnetic system on the coefficient for nonmagnetic one. So we obtain magnetic contribution to the self-diffusion coefficient.

We compare theoretical results with the data of computer simulations, and we have a good agreement.

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**#P064 - Fourier transform infrared spectroscopy characterization of Wild Type Beta-2 Microglobulin and DE Loop Mutants in solution, in single crystals and in form of fibrils**

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$\beta$ -2 microglobulin ( $\beta$ 2m) is an amyloidogenic protein involved in the dialysis related amyloidosis.

Here, we characterized by Fourier transform infrared (FTIR) spectroscopy the wild type protein and its mutants Asp59Pro, Trp60Gly, and Trp60Val. Although they displayed very similar 3D structures, the FTIR measurements in solution pointed to significant differences in thermal stability and aggregation propensity. To comprehend these features, we studied each  $\beta$ 2m variants in form of single crystals by FTIR microscopy. Significant spectral differences were observed between the protein in solution and in the crystalline state involving mainly the main  $\beta$ -sheet band. Furthermore, appreciable differences in secondary structures were found among the variants [1].

We investigated also the  $\beta$ 2m fibrils obtained after incubation for one week of each variant under fibrillogenic conditions. Attenuated total reflection (ATR) measurement displayed a comparable hydrogen/deuterium exchange behaviour of the intermolecular  $\beta$ -sheets, indicating similar accessibility and dynamics of these structures [2].

This study illustrates the potential of FTIR (micro)spectroscopy to obtain complementary structural information on the protein under different physical states, namely in solution, in form of insoluble aggregates, and as single protein crystals.

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#### #P065 - Core placement and faceting in free and supported nanoalloys

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In binary non-miscible nanoalloys, size-mismatch and differences in surface energy often lead to core-shell structures. The structural details of these nanoalloys, such as the position of the core and the thickness of the shell are known to affect in a significant way the properties of the NPs. The subject of our study is determining the placement of the core and the faceting at the core-shell boundaries.

We present an atomistic investigation on the energetics of different core shape and placements in core-shell nanoalloys, considering both free and oxide-supported nanoparticles. Our results show that

(a) There is a universal trend in preferential faceting, that is open-packed (100) or close-packed (111) dominated interfaces, correlated to size mismatch. Since strong strain builds up at interfaces, the simple picture of the Wulff-construction is not valid. This result can be explained through structural relaxation processes common to all systems analysed, having thus a general character indicating its validity to other systems where Wulff theorem fails.

(b) On both free and supported nanoalloys, there is a tendency for the asymmetric placement of the cores. In supported nanoalloys, the core surface may appear at the interface with the oxide, as it happens for Ag-Cu and Ag-Ni on MgO(001).

#### #P066 - Computational investigation of the halloysite nanotube structure

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Thanks to its peculiar tubular shape, halloysite (a 1:1 aluminosilicate with stoichiometry  $\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4 \cdot 2\text{H}_2\text{O}$ ) is considered a promising entrapment system for loading, storage and controlled release vehicle for various species. Economically viable and environmentally friendly, this material is competitive with other tubular systems as carbon, polymeric, metal or metal oxide nanotubes.

In this report the results of a self consistent charge density functional tight binding investigation on models of spiral halloysite nanotubes are shown. This study was aimed to obtain information on the distortions of the kaolinite sheet in the process of nanotube formation, on the nature of the interarms interaction and on the general structural properties of the stoichiometric water molecules in this spiral aluminosilicate. When the properties of the spiral nanotube are compared with those of the kaolinite sheet, a certain degree of intrinsic disorder in the halloysite systems is revealed, due to the intrinsic nature of the spiral folding. This is particularly evident in the hydrogen bonds network occurring in the hydrated nanotube.

The spiralization of a kaolinite sheet, both in the anhydrous and in the hydrated form, does not seem to cause major distortions of the aluminium and silicon polyhedra. In view of this, spiralization of kaolinite should not be an energetically demanding task, in particular when water molecules act as linkages between the spiral arms. The missing periodicity of the unit cell in a spiral nanotube reflects in a large number of possible hydrogen bond geometries, corresponding to just as many minima in the potential energy surface of the nanotube. This would suggest, if the transition from an energy minimum to another is hypothesized effortless,



that the water molecules between the spiral arms are quite unsettled, so that the interaction between the arms could be seen as a dynamic linkage instead of a static one.

#### #P067 - Fabrication and Characterisation of Titania Photonic Nanostructures

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Titanium dioxide is a versatile material, employed in a wide range of applications, including photovoltaic devices, energy storage and photocatalysis. In particular, in recent years  $\text{TiO}_2$  has been incorporated effectively as scaffold layer in organo-halide perovskite solar cells, in which its porosity and meso/nanostructural arrangement play an important role in the charge transport processes occurring in such promising class of photovoltaic devices. It is thus essential to investigate the experimental parameters controlling its structural and optical features.

In this work, we report about the preparation and morphological characterization of photonic nanopatterned titania films (~ 200 nm). These monolayers were prepared via a three-steps method: i) deposition of self-assembled hexagonal closed-packed monolayers of polystyrene microspheres, ii) infiltration of the titanium precursor into the interstitial spaces of the structure and iii) removal of the colloidal crystal template by calcination. Interestingly, by simply using two different deposition techniques during the infiltration step, namely spin-coating and drop-casting, we observe the development of two distinct photonic nanostructures, honeycomb-like lattice and an hexagonal-closed packed microsphere monolayer, respectively. Titania-based nanophotonic structures might be integrated in a number of optoelectronics devices to boost their performances, i.e. as a light-trapping layer in solar cells.

#### #P068 - Properties of the $(\text{Ga}(1-x)\text{In}(x))_2\text{O}_3$ alloy over the whole composition range

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Using density-functional ab initio techniques, we provide the first assessment of the main properties of the increasingly popular  $(\text{Ga}_{1-x}\text{In}_x)_2\text{O}_3$  alloy over the whole range of composition. The alloy is isostructural at low  $x$  with beta- $\text{Ga}_2\text{O}_3$  and at high  $x$  with bixbyite  $\text{In}_2\text{O}_3$ , and exhibits a large and temperature-independent miscibility gap, between approximately 15 and 55% In content for the bixbyite alloy grown epitaxially on  $\text{In}_2\text{O}_3$ , and 15 to 85% for the free-standing bixbyite alloy. The gap, volume and band offsets to the parent compounds also exhibit anomalies as function of  $x$ . Specifically, the offsets in epitaxial conditions are predominantly type-B staggered, but have opposite signs in the two end-of-range phases.

#### #P069 - Behavior of the Berry phase in gapped graphene

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We show that, when a gap of tunable size opens at the conic band intersections of graphene, the Berry phase does not vanish abruptly, but progressively decreases as the gap increases. Further, the phase also depends on the reciprocal-space path radius, i.e., for a doped system, the Fermi wave vector. The phase and its observable consequences can thus be tuned continuously via gap opening –by a modulating potential induced by strain, epitaxy, or nanostructuring– and doping adjustment.

#### #P070 - Absorption anisotropy in $\text{Ga}_2\text{O}_3$ : a joint theory-experiment assessment

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We revisit the issue of optical absorption anisotropy in the monoclinic insulator  $\beta\text{-Ga}_2\text{O}_3$  combining accurate optical absorption measurements with a theoretical analysis performed using different advanced computation methods based on density-functional theory including hybrids, self-interaction correction and GW. As expected, the bandgap edge of bulk  $\beta\text{-Ga}_2\text{O}_3$  is found to depend on the polarization of light and on crystal orientation, with the lowest onset occurring at polarization in the ac crystal plane around 4.5-4.6 eV. Polarization along b unambiguously shifts the onset up by 0.2 eV. The theoretical analysis clearly indicates that the shift of the b onset is due to a suppression of the transition matrix elements of the three top valence bands at  $\Gamma$  point.

**#P071 - Qualitative and quantitative characterization of historical pigments by XRF spectrometry**

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In the Cultural Heritage field, the study of the pigments covers a crucial role, both for historical-artistic and diagnostic reasons; indeed most of the historical paints are mainly constituted by inorganic pigments, either pure or mixed, spread on the surfaces using different binding agents [1]. The knowledge of the exact amount of different constituents of the paint, as well as of the mixing and pictorial techniques, is crucial for a careful program of conservation of polychrome works. Moreover, since the availability of these pigments has been changing through the centuries, their identification and chemical characterisation is useful to acquire or deepen information about the artist and his/her work. This information can also be useful for authentication purposes through relative dating because the identification of one pigment respect to another one can be used as a *terminus post quem* or *ante quem* the artwork was realized.

On the basis of the before considerations, this work is focused on the chemical characterization and quantitative analysis of binary mixtures obtained by mixing historical pigments: cinnabar, lapis lazuli, lead-tin yellow and chalk white. They were analysed both in pure and mixed form, by varying their weight percentage, in order to produce binary mixtures [2] (realized following the Itten Theory and the ancient artists recipes) to be investigated by means of a portable XRF spectrometer in order to carry out qualitative and quantitative analyses of the two pigments constituent the mixture [3].

This experimental approach allows calculating the weight percentage of the single component, on an unknown (for the analyst) mixture, composed by two known pigment, by inverse prediction on the calibration curve.

**#P072 - Facile growth and transfer of high quality graphene layers by simple thermal treatments**

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Graphene growth is nowadays achievable by a wide variety of techniques. We demonstrate the possibility to grow high quality graphene single and few layers by using simple and economic UHV thermal treatments of thin (100-150 nm thick) nickel films deposited on Si/SiO<sub>2</sub> (300 nm) substrates and nickel foam. The crucial role played by process parameters to trigger the graphene growth yield as well as the overall film quality has been extensively investigated. In particular, hypothesis on the growth mechanism is given in comparison with literature reports, with particular attention devoted to the effect of external carbon sources and process pressure on single layer growth. Raman mapping confirms the presence of domains of turbostratic multi-layer areas as well as single layer graphene islands as large as several  $\mu\text{m}$ . SEM and AFM analyses allow for a detailed morphological characterization of nickel film after annealing process and the observed anomalous grain growth seem to be correlated to graphene formation. The as grown graphene layers can be further transferred onto any kind of substrate by wet methods. We conclude that UHV annealing of nickel film and foam represent a valuable approach to provides graphene-based materials for sensors and devices.

**#P073 - Multiphoton k-resolved photoemission from gold surface states with 800-nm femtosecond laser pulses**

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We measure direct multiphoton photoemission of the Au(111) surface state with 800-nm laser pulses. We observe the parabolic dispersion in the angular distribution of photoelectrons having absorbed between four and seven photons. The  $k_{\parallel}$  dispersion we measure can be explained in terms of Shockley-state replicas, with a nascent hot electrons distribution at  $k_{\parallel}$  above the Fermi level. Moderate laser power densities, of the order of  $100\text{GW}/\text{cm}^2$ , resulted in large electron yields, indicating the importance of multiphoton excitations to define the electronic and magnetic properties of matter in the first hundred femtoseconds after laser excitation [[Phys. Rev. B 2014, 90, 035401](#)].

**#P074 - Enhanced Atom Mobility on the Surface of a Metastable Film**

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A remarkable enhancement of atomic diffusion is highlighted by scanning tunneling microscopy performed on ultrathin metastable body-centered tetragonal Co films grown on Fe(001). The films follow a nearly perfect layer-by-layer growth mode with a saturation island density strongly dependent on the layer on which the nucleation occurs, indicating a lowering of the diffusion barrier. Density functional theory calculations reveal that this phenomenon is driven by the increasing capability of the film to accommodate large deformations as the thickness approaches the limit at which a structural transition occurs. These results disclose the possibility of tuning surface diffusion dynamics and controlling cluster nucleation and self-organization [Phys. Rev. Lett. 2014, 113, 046102](#).

**#P075 - High resolution NEXAFS of perylene and PTCDI: a surface science approach to molecular orbital analysis**

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We made use of synchrotron radiation to perform near edge X-ray absorption fine structure spectroscopy, NEXAFS, at the carbon K-edge of perylene and perylene-tetracarboxylic-diimide, PTCDI. Reference spectra measured for isolated molecules in the gas phase are compared with polarization dependent NEXAFS spectra measured on highly oriented thin films in order to study the symmetry of the molecular orbitals. The molecular overlayers are grown onto the rutile TiO<sub>2</sub>(110) surface for which the large anisotropic corrugation effectively drives the molecular orientation, while its dielectric nature prevents the rehybridization of the molecular orbitals. We employed density functional theory, DFT, calculations to disentangle the contribution of specific carbon atoms to the molecular density of states. Numerical simulations correctly predict the observed NEXAFS azimuthal dichroism of the  $\sigma^*$  resonances above the ionization threshold, from which we determine the full geometric orientation of the overlayer molecules. A discrepancy observed for the spectral contribution of the imide carbon atom to the calculated unoccupied molecular orbitals has been explained in terms of initial state effects, as determined by Hartree–Fock corrections and in full agreement with the corresponding shift of the C 1s core level measured by X-ray photoelectron spectroscopy, XPS. [Phys. Chem. Chem. Phys., 2014, 16, 14834-14844](#)

**#P076 - Anchoring and Bending of Pentacene on Aluminum (001)**

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The adsorption of the first layer of organic molecules at the metal–organic interface in electronic devices is critical as it influences the carrier injection across the interface and also forms the foundation for the growth of the subsequent layers, which in turn affects the overall performance of these devices. Pentacene (C<sub>22</sub>H<sub>14</sub>) has shown temperature-independent highest hole and electron mobility among the various organic small molecules. Aluminum is also a metal of potential interest for Si-free electronic devices. Pentacene coupled to aluminum could be used to fabricate devices like Schottky diodes and organic thin film transistors, and the interaction between pentacene and aluminum is also important in organic solar cells and memory devices.

In our study of pentacene/Al(001), we combined ab initio simulations, based on density functional theory (DFT) corrected for the van der Waals interaction, with techniques to determine the structure of the system, such as reflection high-energy electron diffraction (RHEED) and scanning tunneling microscopy (STM) and core-level spectroscopies, namely X-ray photoemission spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) [1].

We find a major change of the molecular backbone resulting into a peculiar V-shape bending, due to the direct anchoring of the two central carbons atop two Al atoms underneath. In the most stable adsorption configuration, pentacene is oriented with the long axis parallel to the substrate [110] direction, where such anchoring is favored by optimally matched interatomic distances. Remarkably, due to the generally low degree of order, we measure by STM a significant portion of molecules oriented along the [100] direction, which also display the same V-shape conformation, as driven by the bond of the central carbon atoms of pentacene

to a pair of slightly displaced Al atoms. Even in absence of long-range order, the substrate thus favors a specific structural and electronic molecular conformation, which can be representative of a real interface layer of pentacene at an Al electrode.

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#### #P077 - Quantum ring: HHG spectrum control.

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Atoms, molecules, clusters and other systems driven by a strong laser field of frequency  $\omega_L$  can emit a spectrum of laser harmonics.

The high harmonics generation (HHG) phenomenon is strongly affected by the symmetries of the system. It is well known that systems with rotational symmetries emit only odd harmonics.

Numerous researchers make mainly attention to the possibilities to set different initial conditions in order to control the spectrum.

Recently, the study of nanotechnology is hot-topics and in particular the study of very symmetric systems such as fullerene, nanoring and structured nanoring (nanoring with identical and symmetric scattering centers).

Therefore, it is natural and interesting to study the HHG emission from these systems and the effects of the symmetry break.

In this poster we present the HHG spectrum emitted by a nanoring consisting of six symmetric scattering centers; as a second step we study the effects on the spectrum by small symmetry breakings. We show that tiny modifications of the symmetry allow a good control of the spectrum.

#### #P078 - ON SURFACE DATING OF BRICKS

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Luminescence techniques are nowadays a powerful tool to date archaeological ceramic materials and geological sediments. In particular thermoluminescence (TL) is widely used for brick dating, to reconstruct the building chronology of urban complexes. However, it can be sometimes inconclusive, since TL assesses the firing period of bricks, that can be reused in different structures even after centuries. This problem can be circumvented by using a dating technique which uses a resetting event different from that of TL, which is the last heating of the material. An ideal candidate is OSL, for which the reset is the last exposure to sun light. In fact, the exposure of the brick surfaces during the edification resets the light sensitive electron traps until the covering with mortar. This advanced application of the OSL technique (surface dating) has been successfully attempted on rocks, marble and stone artifacts, but not routinely on bricks. An attempt of application was possible thanks to a recent conservation campaign at the Certosa di Pavia complex (Italy) where some bricks belonging to a XVII century collapsed wall could be sampled. It was therefore possible to compare the dating results obtained by TL and OSL with the historical data. The main requirement for the successful application of surface dating is the assessment of the bleaching effectiveness of the solar exposure. To evaluate the sunlight effects on the luminescence signal of the surface, small carrots of brick have been exposed to daylight for different periods (from 60 s to 1 year). Measurements of the OSL/IRSL signals showed that after a few hours the signal from the surface was reduced to 20% of the original one. The deeper layers were significantly bleached only after one month of exposure. The depth profile of signals (OSL emission vs. depth) depends on the opacity of the material, on the daylight spectrum and on the exposure time. The characteristic form of the OSL/IRSL resetting profile in a brick is well fit by an empirical mode based on that proposed for rocks [Sohbati et al., 2012], adding a time-dependent exponential term to the function of light signal vs depth.

R. Sohbati *et al.*, *J. Geophys Res-Sol* 117 (2012).

#### #P079 - Proposal of a method for correcting the dose images measured with gafchromic EBT3 films irradiated with proton beams

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The response of gafchromic EBT3 films depends on the LET of radiation, showing a quenching effect in the high LET region. A method has been studied to correct the measured values in a simple and efficient way, feasible in the clinical practice. Considering that for patient treatments hundreds of beams are necessary, two points were taken as a basis of the procedure to be developed. The first point was that of avoiding the measurement of the depth-dose curve for all the utilized energies, evaluating the function

vs depth of both the depth-dose curve and the curve of under-response, utilizing the data measured with a few energies in the range of those exploited for the treatment. The second point was that of utilizing the treatment plane data as input of the software developed for the correction procedure. In order to correct the acquired images not only in SOBP condition but also for non-uniform dose distributions, the software evaluates a correction factor, in each position of the image, utilizing algorithms that take into consideration the contributions of each pencil beam of the performed irradiation that can contribute to the absorbed dose in the considered point.

The software for the image correction, developed in MATLAB, is still in improvement. The first results confirm that the proposed method can be advantageous for achieving reliable spatial distribution of the absorbed dose in proton therapy by means of EBT3 films. The method deserves to be exhaustively improved by means of more precise evaluation of the broadening of pencil beams in tissue or in water. The developed software will be then suitably adjusted in order to be applicable also to radiotherapy with carbon ions.

#### #P080 - Ta-doped Bi<sub>2</sub>O<sub>3</sub> investigated with X-Ray Absorption Spectroscopy and Density Functional Theory

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The design of efficient anion conducting IT-SOFC, working between 500-800°C, is a currently open challenge for the production of clean power from H<sub>2</sub> or biofuel. [1] One of the critical parameters in the development of this technology is the anion diffusion inside the electrolyte. The conduction mechanism is in turn determined by the local environment of cations involved in the process of anion diffusion, and to this end X-Ray Absorption Spectroscopy (XAS) represents a powerful tool to resolve the finer details of the atomic structure. Moreover, a Density Functional Theory (DFT) approach is extremely useful to identify the energetically favourite atomic configurations. Today, cubic fluorite-type  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> represents the reference compound for the design and optimization of new electrolytes, as it shows the highest oxide-ion conductivity known so far (1 S cm<sup>-1</sup> at 750°C). Unfortunately, pure  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> is thermodynamically stable only in a narrow temperature range, but the structure can be stabilized by insertion of different dopants. [2]

We have recently studied Bi<sub>2</sub>O<sub>3</sub>-Ta<sub>2</sub>O<sub>5</sub> solid solutions in the concentration range between 7.5 and 30%mol by means of XAS, to shed light on the local structure around cations. Extended X-Ray Absorption Fine Structure (EXAFS) data analysis on Bi L<sub>3</sub>-edge reveals a highly disordered environment around bismuth. In particular, the presence of two different first shell distances Bi-O, suggests that oxygen ions are displaced from the centroid of their OB<sub>4</sub> coordination tetrahedron. [3]

Concerning the local environment of dopants, the results on the Ta L<sub>3</sub>-edge are consistent with an octahedral coordination around Ta, forming TaO<sub>6</sub> units. Below 10%mol, Ta forms isolated TaO<sub>6</sub> octahedra, while between 10 and 30%mol, the TaO<sub>6</sub> octahedra are locally organized in Ta<sub>7</sub>O<sub>30</sub> clusters, arising from corner-sharing TaO<sub>6</sub> octahedra, which resemble the pyrochlore structure. These clusters tend to aggregate further as the dopant concentration increases, and this evidence is corroborated by the high Ta-Ta coordination numbers, between 3.1 and 3.9.

Finally, periodic DFT optimizations, performed on Bi<sub>0.75</sub>Ta<sub>0.25</sub>O<sub>1.75</sub> with the CRYSTAL09 code, strongly support the experimental evidence on the aggregation of Ta clusters at high dopant concentration. Indeed, comparing the energy values for the i) isolated clusters and ii) linked clusters configuration, it is found that the linked clusters model has the lowest energy. These result support the EXAFS experimental results and justify the high Ta-Ta coordination numbers found in the Ta-doped samples.

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#### #P081 - Fundamental study and analytical applications of Nanoparticle-Enhanced LIBS (NELIBS).

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Nanoparticle-Enhanced LIBS (NELIBS) is a recently proposed method to efficiently increase the LIBS emission signal of metals up to 2 orders of magnitude, by depositing metal nanoparticles (NPs) on the sample surface [1]. This considerable emission enhancement has been ascribed to two effects: 1) an improvement in the ablation effect, and 2) a more efficient production of seed electrons by field emission, in turn due to the enhancement of the laser electromagnetic field induced by the NPs themselves [2].

Here, we report our investigations about the effect played by several experimental parameters, i.e., laser energy; laser spot diameter; concentration, dimension, and kind of nanoparticles (NPs) in the case of NELIBS of metals. We also discuss NELIBS of non-metallic samples, whose emission enhancement is lower (up to 2-3 times) and follows a different mechanism. A special case of particular interest is that of transparent media, which can be efficiently made more absorptive by NP deposition. Moreover, we demonstrated the suitability of NELIBS to quantitative analysis of various samples (metals, alloys and non-metallic samples), both with the classical approach of drawing calibration lines and with calibration-free methods.

- [1] A. De Giacomo, R. Gaudiuso, C. Koral, M. Dell'Aglio, O. De Pascale, *Nanoparticle-Enhanced Laser Induced Breakdown Spectroscopy of metallic samples*, Analytical Chemistry, 85 (2013) 10180-10187.
- [2] A. De Giacomo, R. Gaudiuso, C. Koral, M. Dell'Aglio, O. De Pascale, *Nanoparticle Enhanced Laser Induced Breakdown Spectroscopy (NELIBS): effect of nanoparticles deposited on sample surface on laser ablation and plasma emission*, Spectrochimica Acta B, 98 (2014) 19-27.

#### #P082 - Spin-Crossover Molecule based Thermoelectric Junction

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Using *ab-initio* numerical methods, we explore the spin-dependent transport and thermoelectric properties of a spin-crossover (SCO) molecule (i.e. iron complex of 2-(1H-pyrazol-1-yl)-6-(1H-tetrazole-5-yl)pyridine) based nano-junction. We demonstrate a large magnetoresistance, efficient conductance-switching and spin-filter activity in this molecule based two-terminal device. The spin-crossover process also modulates the thermoelectric entities. It can efficiently switch the magnitude as well as spin-polarization of the thermocurrent. We find that thermocurrent is changed by ~4 orders of magnitude upon spin-crossover. Moreover, it also substantially affects the thermopower and consequently, the device shows extremely efficient spin-crossover magnetothermopower generation. Furthermore, by tuning the chemical potential of electrodes into a certain range, a pure spin-thermopower can be achieved for the high-spin state. Finally, the reasonably large values of figure-of-merit in the presence and absence of phonon, demonstrate a large heat-to-voltage conversion efficiency of the device. We believe that our study will pave an alternative way of tuning the transport and thermoelectric properties through the spin-crossover process and can have potential applications in generation of spin-dependent current, information storage and processing.

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#### #P083 - BSA hydrogels: a novel biomaterials

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Recently the fabrication of gels from biological molecules has received increasing interest in the field of biomaterials. Indeed these gels, especially the hydrogels, can be biocompatible and biodegradable, can entrap large amounts of water or biological fluid, have a microporous structure and provide an excellent mechanical support through their three-dimensional structure. These properties make them the ideal biomaterials for applications in the biomedical field.

Here we report our results, obtained exploiting the proteins' natural tendency to self-organize in a 3D network, for the production of new protein-based materials. The main aim of our work has been to determine the best experimental conditions to obtain a hydrogel of protein aggregates of BSA, a human-compatible and well-known protein. Our experimental procedure was to characterize the nature of the aggregates created at different pH and the mechanical properties of the gel formed during the incubation time; finally we tested the obtained protein hydrogels on a cellular model to verify their application as 3D scaffold.

We analyzed the conformational and structural changes of the protein during all the steps of the thermal aggregation and gelation through FTIR and AFM measurements. The macroscopic hydrogel features have been tested by rheological measurements. SEM images have given a picture of the different arrangement of the protein aggregates created at different pH at the end of the incubation time. Biological tests on LAN5 cell culture have been performed. Our results indicate that BSA hydrogels can be a promising material for biological application in the field of tissue engineering.

#### #P084 - Degradation of Cd-yellow Paints induced by adsorption of water and oxygen on CdS surface. Ab initio approach

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The cadmium yellow paints (CdS) used in impressionist and modernist paintings in early 1900s are undergoing several deterioration processes whitening and discoloration. This discolored crusts at the surface of the paintings is formed mainly by white globular hydrated cadmium sulfate ( $\text{CdSO}_4 \cdot n\text{H}_2\text{O}$ ) and cadmium carbonate ( $\text{CdCO}_3$ ). The input for the formation of such whitish compounds

is generally ascribed to an initial photo-oxidation process of Cd-yellow or to products used during the syntheses of CdS.[1] Also, structural defects in CdS (deep traps) may play a role in the pigment alteration process

In order to understand the oxidation and hydration mechanisms of the whitish globules, at atomic level, we present a theoretical study of point defects, namely Cd- and S- vacancies, both in the bulk and in the hexagonal non-polar {10.0} surface. The interaction between the {10.0} defective surface of CdS and O<sub>2</sub> and H<sub>2</sub>O molecules is then studied to simulate the combined effects of exposure to air and humidity. For this purpose, we adopted a first principles method within the framework of the Density Functional Theory (DFT) in the Generalized Gradient Approximation (GGA-PBE) with the use of ultrasoft pseudopotentials. [2]

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### #P085 - “Darker-than-Black” PbS Quantum Dots: Enhancing Optical Absorption of Colloidal Semiconductor Nanocrystals via Short Conjugated Ligands

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Here we present a conceptually novel approach to design light-harvesting nanomaterials based on colloidal quantum dots (QDs). Indeed, a drastic broadband enhancement of QD optical absorption, along with preservation of good long-term colloidal stability, is obtained upon quantitative replacement of the bulky electrically-insulating ligands at the QD surface coming from the synthetic procedure with suitable short conjugated organic molecules. The rational design of the pendant and anchoring moieties that constitute the replacing ligand framework provides tunable broadband increase of the optical absorption above 300 % for colloidal PbS QDs also at high energies (> 3.1 eV), in contrast with predictions obtained by established formalisms derived from Maxwell-Garnett effective medium theory. We attribute such a drastic absorbance increase to ground-state ligand/core orbital mixing, as inferred by density functional theory calculations; in addition, our findings suggest that the optical bandgap reduction commonly observed for PbS QD solids treated with thiol-terminating ligands can be prevalently ascribed to 3p orbitals localized on anchoring sulfur atoms, which mix with the highest occupied states of the PbS core.

More broadly, we provide evidence that organic ligands and inorganic cores are inherently electronically coupled materials thus yielding peculiar chemical species (the colloidal QDs themselves), which display arising (opto)electronic properties that cannot be merely described as the sum of those of the ligand and core components.

### #P086 - Variants of Intrinsic Disorder among Human Disease-related Proteins

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Intrinsically disordered proteins are fascinating the community of protein science, at least since the last decade. There is a well-established line of research that intends to reveal the crucial role played by intrinsically disordered proteins (IDPs) in the development of human diseases. The main argument is that IDPs are differentially more present in groups of disease-related proteins. In this work we revisit a theme which has been quite present in the specialised recent literature, that of the differential occurrence of disordered proteins among groups of disease-related proteins in the human proteome. Distinguishing two variants of disordered proteins (those with long disordered domains or regions (IDRs), the others with both localised disorder and wide-spread intrinsic disorder (IDP) clarifies to which extent there is a differential enrichment of disorder among proteins that pertain to cancer, diabetes cardiovascular and neurodegenerative diseases. In particular, disease-related proteins are enriched in IDRs but not in IDPs.

### #P087 - An “optimal” protein– saccharide ratio for bioprotection is present in low hydration amorphous saccharide glassy systems: a FTIR study

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Saccharides, and in particular trehalose, are well known for their high efficiency in protecting biostructures against adverse environmental conditions. Experiments and simulations [1] on carboxy-myoglobin (MbCO) have shown that the protein dynamics is highly inhibited in a low-water trehalose host medium, the inhibition being markedly dependent on the amount of residual water. Beside hydration, the properties of the saccharide amorphous matrices are noticeably variable also with the protein/sugar ratio.

In the work here presented, we performed an Infrared Spectroscopy (FTIR) study on the stretching band of the bound CO molecule (COB) and on the Water Association Band (WAB) in dry amorphous matrices of various sugars (the disaccharides trehalose, maltose, sucrose and lactose, and the trisaccharide raffinose), at different protein/sugar ratios. Such bands have already been successfully exploited for the simultaneous study of the thermal evolution (20-300K) of the embedded biostructure and of the matrix; indeed, the COB is one of most studied protein spectroscopical marker, and the WAB a very sensitive probe for the low-water matrix.

The results show a high dependence of the protein and matrix dynamics on the protein/sugar ratio, depicting a scenario in which the system dynamics evolves from matrix-slaved to coupled and eventually to protein slaved, with increasing protein concentration. This supports the idea, already proposed [1,2], that a mutual protein $\rightleftharpoons$ matrix structural and dynamic influence subsists in low hydrated systems, indicating that the protein-solvent master and slave paradigm does not strictly hold, but the mutual relationship depends on the relative concentrations. Furthermore, for each sugar, an optimal protein/sugar concentration ratio, which maximizes the protein preservation minimizing the thermal dynamics, can be identified.

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### #P088 - Noisy dynamics in long and short Josephson junctions

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The transient dynamics of different noisy *Josephson junctions* (JJ) are computationally explored, analyzing several interesting cases. First, the superconducting lifetime of a long JJ (LJJ) is investigated, analyzing its behavior as a function of the system and noise parameters. Specifically we study the dynamics of the parameter  $\varphi$ , i.e. the phase difference between the macroscopic wave functions in the two electrodes of the junction, whose dynamics is ruled by the *perturbed sine-Gordon* (SG) equation. We focus on the *mean switching time* (MST), calculated as a *nonlinear relaxation time*, from the superconducting metastable state to the resistive state. The dynamics of the phase difference  $\varphi$  is studied in the presence of an external noise source, modeled by using different  $\alpha$ -stable (or Lévy) distributions  $S_\alpha(\sigma; \theta; \mu)$ . For proper values of the system parameters and different statistics of the noise source, the MST is characterized by non-monotonic trends. The study of the time evolution of  $\varphi$  highlights the influence of noise induced *solitons* on the MST behavior. In the presence of the so-called *Lévy flights*, another localized SG solutions, known as *breathers*, can be detected.

The features of a ballistic *graphene-based* JJ is also investigated. The phase dynamics of this system is analyzed by the *Resistively and Capacitively Shunted Junction* model, with a thermal noise contribute. The supercurrent deviates from the usual sinusoidal behavior expected from the Josephson relations. A *superconductor-graphene-superconductor* system is characterized, as normal current biased JJs, by the presence of quantum metastable states. In our work, the *mean first passage time* (MFPT) from these metastable states is calculated in the presence of different sources of white or correlated Gaussian noise. MFPT data are obtained for different values of both noise intensity and frequency of the alternate current bias, observing noise induced phenomena. The study of the *probability density function* of the escape times is performed, by focusing on the appearance of noise induced non-monotonic effects in the mean switching times.

We also present a study on the exclusive breather generation in LJJ stimulated by an external driving signal. This study is devoted to establish an efficient experimental setting to generate SG breathers in a LJJ, exploiting a well-known phenomenon, the *nonlinear supratransmission* (NLS). In our model, one end of the junction is driven by a sinusoidal pulse of amplitude  $A$  and frequency  $\omega$  lower than the plasma frequency of the junction. In the 2D parameter space  $(A, \omega)$ , in correspondence of specific values of  $A$  and  $\omega$ , we observe only breathers. Otherwise, different combinations of SG solutions propagate along the junction. To check the robustness of the breathers generated, a Gaussian noise source is inserted into the perturbed SG model, and the percentage of surviving breathers is calculated.

### #P089 - Quality control of foods and nutraceutical applications: antioxidant properties of polyphenols.

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The Mediterranean diet is characterized by an abundance of fruits and vegetables considered nutraceuticals foods. Indeed, due to a high content of polyphenols, fruits and vegetables play an excellent role in maintaining human well-being, enhancing health and



preventing or even treating specific diseases. Polyphenols are a unique group of phytochemicals with substantial healthy potential in many medical areas. Their activity is based on functional groups capable of accepting a free radical's negative charge. The aim of our study was to investigate the possibility of developing a new natural phytoextract, obtained by mixing bioactive components from different Mediterranean species with a potential synergistic bioactive effect. Bioactive molecules, extracted from different Mediterranean species, have been characterized and separated by High Performance Liquid Chromatography. Folin-Ciocalteu, ORAC, DPPH assays were carried out to determine phenolic content and antioxidant capacity. Results have revealed variability in phenolic content and composition among the different tissues and species. The effects of Polyphenol extracts from apple different tissues were analyzed on the NIH-3T3 cell line.

#### #P090 - ARTIFICIAL AGING ON PAINTINGS: A STUDY OF THE CHROMATIC CHANGES

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The colour specification is relevant in the study, the conservation and the restoring of ancient paintings. As is known the colour we see is not always the original one, but it has been subject to different kind of alteration phenomena like the chemical and physical degradation that modify the appearance of the pictorial materials. Every diagnostic program takes into account quantifying the chromatic variation of the artistic artefacts due to the aging and to the exposure to different climatic conditions. The main objective is the prevention of degradation phenomena, so it's necessary to realize studies aimed to the knowledge of materials and the related characterisation. These phenomena are the results of different agents as temperature, humidity and the exposure to light during many years. The artificial aging techniques can reproduce, in laboratory, the effect of time in a short period. In this way it is possible to study selectively the effects of the degrading agents and the modification of the optical and physical characteristics. The aim of this work is the quantification, by optical reflectance spectroscopy, of the chromatic variation on paintings after different cycles of controlled artificial aging, on varying temperatures and humidity (thermo-hygrometric aging) and modifying the exposure to optical radiation (induced photo-degradation). For this purpose, a climatic room able to change simultaneously temperature, relative humidity, light, Ultraviolet (UV) and Infrared (IR) radiations exposure was used. Photo-degradation was evaluated separately in a Lighting box equipped with five different sources: D65 (Artificial Daylight), 840 (formerly TL84), F (Point of Sale lamp), Tungsten Filament (typical home lighting) and UV (Ultra Violet Blacklight). The aging cycle was performed varying temperature, relative humidity and exposure to electromagnetic radiation in the climatic room. The effects of the photo-degradation after the exposure to different radiation sources in the Lighting box were also evaluated. The measurements were performed on painting samples specifically prepared with historical pigments of different hues (blue, green, red and yellow) painted using four different binders (Casein, Linseed Oil, Poppy Oil and Egg yolk) in order to evaluate the role of medium. The same aging cycle was applied on every pigment painted with all binders and the effects were measured with the routine protocol for the optical reflectance spectroscopy. The results were analyzed comparing the Spectral Reflectance Factor (SRF%) trend and the chromatic coordinate values in the CIE Lab color space. The role in the artificial aging process of each binder and each pigment powder was also evaluated.

#### #P091 - Condensed phase of Bose-Fermi mixtures with a pairing interaction

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We study the condensed phase of a Bose-Fermi mixture with a tunable pairing interaction between bosons and fermions with many-body diagrammatic methods and fixed-node diffusion quantum Monte Carlo simulations. For a 3D system, a universal behavior of the condensate fraction and bosonic momentum distribution with respect to the boson concentration is found to hold in an extended range of boson-fermion couplings and concentrations. For vanishing boson density, we prove that the bosonic condensate fraction reduces to the quasiparticle weight  $Z$  of the Fermi polaron studied in the context of polarized Fermi gases, unifying in this way two apparently unrelated quantities. For the 2D case we present some preliminary results in the weak-coupling limit for chemical potentials and condensate fraction.

#### #P092 - Band-edge BCS-BEC crossover in a two-band superconductor: physical properties and detection parameters

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Superconductivity in iron-based magnesium diborides and other novel superconducting materials has a strong multi-band and multi-gap character. Recent experiments support the possibility for a BCS-BEC crossover induced by strong-coupling and proximity

of the chemical potential to the edge of one of the bands. Here we study the simplest theoretical model which accounts for the BCS–BEC crossover in a two-band superconductor, considering tunable interactions and tunable energy separations between the bands. Mean-field results for condensate fraction, correlation length, and superconducting gap are reported in typical crossover diagrams to locate the boundaries of the BCS, crossover and BEC regimes. When the superconducting gap is of the order of the local chemical potential, superconductivity is in the crossover regime of the BCS–BEC crossover and the Fermi surface of the small band is smeared by the gap opening. In this situation, small and large Cooper pairs coexist in the total condensate, which is the optimal condition for high- $T_c$  superconductivity. The ratio between the gap and the Fermi energy in a given band results in the best detection parameter for experiments to locate the system in the BCS–BEC crossover. Using available experimental data, our analysis shows that iron-based superconductors have the partial condensate of the small Fermi surface in the crossover regime of the BCS–BEC crossover, supporting the recent ARPES findings.

#### #P093 - Glycation effects on the conformational properties and fibrillization of $\beta$ -lactoglobulin

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The glycation process, by Maillard reaction, involves the interaction of reactive side chain amine groups (lysine, arginine and N-terminal) of proteins with the carbonyl groups of sugars. The final product of the reaction is a family of heterogeneous compounds called Advanced Glycation End products (AGEs), which play an important role in aging processes and neurological disorders.

We report on the effects of different degree of glycation of  $\beta$ -lactoglobulin (BLG) with glucose and dihydroxyacetone (DHA) on the conformational and aggregation properties of the protein, by combining different experimental approaches. Glycation was performed in the dry state by incubating samples at 40 °C for different times (8 and 72 h for glucose, 2, 4, 8 and 72 h for DHA). A mixture of BLG glycoforms was identified by mass analysis, with an average of 3 and 10 modified sites after, respectively, 8 and 72 h of incubation with glucose. In contrast, DHA is more effective to trigger the reaction, and 12 glycation sites were observed after only 2 h of incubation.

Formation of AGEs was monitored by fluorescence spectroscopy, and two different compounds were formed, pentosidine and malondialdehyde, whose concentration increases with the glycation degree.

Glycated BLG shows a marked reduction in the binding affinity for stearic acid at high glycation levels. This finding suggests that one or both lysine residues anchoring the fatty acid could be involved in the glycation process, altering the functional properties of the protein.

Fibrillization induced by high temperature incubation at low pH of glycated BLG was characterized by AFM, FTIR, NMR, WAXS. The overall results show that the fibrils produced by glucosylated BLG are formed by short glycated peptide sequences and are more flexible compared to those formed by the native protein. Sporadic and even shorter fragments are present when BLG reacts with DHA.

The energetics of the fibrillation process investigated by DSC shows an exothermic profile for glucosylated BLG, typical of self-assembled  $\beta$ -structured fibrils, even if less marked compared to the unmodified protein. Interestingly, the exothermic peak is absent for BLG glycated with DHA.

To conclude, both sugars bind to the protein residues and exert a steric hindrance affecting both the protein functionality and the morphology of the resulting aggregates.

#### #P094 - Radiative Near field Heat transfer

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We study radiative (near field) heat transfer between objects in vacuum at different temperatures. By use of classical scattering theory[1], we derive closed expressions for this transfer for objects of arbitrary shape and material, from which general properties of the transfer can be analyzed. We present several examples including spheres, cylinders and ellipsoidal particles[2], thereby demonstrating the size and shape dependence of radiative heat transfer.

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#### #P095 - Nonlinear quantum transport in molecular junctions: a uniform theory bridging coherent tunneling and Coulomb blockade limits based on the Anderson's imputiy model

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We develop a novel nonlinear quantum transport theory through molecular junctions in the presence of electron-electron interaction by using nonequilibrium Green's function (NEGF) techniques and renormalized perturbation theory. In the perturbation treatment, the zeroth-order Hamiltonian of the molecular junction is composed of independent single-impurity Anderson's models (SIAMs), which act as the channels where charges come through or occupy, and the interactions between different channels are treated as the perturbation. Within this scheme, the effects of molecule-lead interaction, electron-electron interaction and hopping interaction are included nonperturbatively, and the charge transport process can be studied in the intermediate parameter range from Coulomb blockade regime to coherent tunneling regime. The concept of quasi-particle is introduced to describe the kinetic process of charge transport, and then the electric current through sequential tunneling and coherent tunneling can be distinguished and calculated. As a test study, the Hubbard model is used as the molecular Hamiltonian to simulate dimeric and trimeric molecular junctions. Various nonlinear current-voltage characteristics, including Coulomb blockade, negative differential resistance (NDR), rectification and current hysteresis, are shown in the calculations, and the mechanisms are elucidated.

### #P096 - Fluid theory of the ultrarelativistic regime in the propagation of an ultrastrong, femtosecond laser pulse in a plasma

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The interaction of a multi-petawatt, pancake-shaped laser pulse with an unmagnetized plasma is studied analytically and numerically in a regime with ultrarelativistic electron jitter velocities, in which the plasma electrons are almost completely expelled from the pulse region. The study is applied to a laser wakefield acceleration scheme with specifications that may be available in the next generation of Ti:Sa lasers and with the use of recently developed pulse compression techniques. A set of novel nonlinear equations is derived using a three-timescale description, with an intermediate timescale associated with the nonlinear phase of the electromagnetic wave and with the spatial bending of its wave front. They describe, on an equal footing, both the strong and the moderate laser intensity regimes, pertinent to the core and to the edges of the pulse. These have fundamentally different dispersive properties since in the core the electrons are almost completely expelled by a very strong ponderomotive force, and the electromagnetic wave packet is imbedded in a vacuum channel, thus having (almost) linear properties. Conversely, at the pulse edges, the laser amplitude is smaller, and the wave is weakly nonlinear and dispersive. New nonlinear terms in the wave equation, introduced by the nonlinear phase, describe without the violation of imposed scaling laws a smooth transition to a nondispersive electromagnetic wave at very large intensities and a simultaneous saturation of the (initially cubic) nonlocal nonlinearity. The temporal evolution of the laser pulse is studied both analytically and by numerically solving the model equations in a two-dimensional geometry, with the spot diameter presently used in some laser acceleration experiments. The most stable initial pulse length is estimated to exceed 1.5–2 microns. Moderate stretching of the pulse in the direction of propagation is observed, followed by the development of a vacuum channel and of a very large electrostatic wake potential, as well as by the bending of the laser wave front.

### #P097 - ABSENCE OF RECONFIGURATION FOR EXTREME PERIODS IN RECTANGULAR ARRAYS OF ANTIDOTS

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We study the magneto-resistance oscillations of four reference samples, S1 to S4, with varying periods in rectangular arrays of antidots on superconducting Nb film. Conforming to literature, the oscillations of S1 reveal the existence of two types of matching effect with different constant magnetic field intervals induced by reconfiguration. On the contrary, we observe very sharp and narrow magneto-resistance oscillations in S4 with very small period of antidots, and a maximum of two oscillations in S2 and S3 with large period of antidots, without any reconfiguration. Therefore, we establish that when the period of antidots either approaches zero or becomes very large, the reconfiguration phenomenon vanishes, and only one type of matching may be observed.

Table 1: Geometrical parameters of the various antidot (holes)array samples.

Sample	Antidot array (nm)	Direction of current (nm)	Diameter of Hole (nm)
S1	400·800	400	200
S2	800·1600	800	200
S3	1600·800	1600	200
S4	300·400	300	290

**#P098 - Thermodynamics and transport properties of high-density hydrogen plasma**

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The development of new technologies and experimental techniques has triggered intensive theoretical research on the modeling of spatially confined quantum systems [1, 2] and also of extreme-high-pressure plasmas [3] like in stellar envelopes [4].

The thermodynamic properties and transport coefficients of non-ideal, high-density hydrogen plasma have been investigated, accounting for quantum effects due to the change in the energy spectrum of atomic hydrogen when the electron-proton interaction is considered embedded in the surrounding particles. High-density conditions have been simulated assuming atomic hydrogen subject to a screened Coulomb potential, to account for the surrounding plasma.

The ionization equilibrium is affected by the pressure ionization phenomenon, deeply investigated in literature as resulting from the non-ideal Debye-Hückel corrections [5]. The influence of the plasma leads to a correction term lowering the ionization potential, that corresponds to the so-called self-energy shift [5,6],  $\Delta = -e^2/\lambda_D$ , thus leading to an effective value  $I_{\text{eff}} = I_0 - \Delta$ , where  $I_0$  is the ionization potential of the isolated, unperturbed hydrogen atom. Actually an additional lowering is due to the effect of the presence of a screened Debye potential on the eigenvalues for electronic levels obtained solving the Schrödinger equation, correspondingly observed in the case of box confinement. Furthermore the ensemble of levels affects also the internal partition function of H atom in the Saha equation.

The effects of non-ideality in the thermodynamics of high-density hydrogen plasma on transport properties have been investigated in the frame of the Chapman-Enskog theory. The electrical conductivity of Debye plasma also exhibits a dependence on the total electron density that is affected by the pressure ionization, i.e. the minimum behavior of the conductivity and the *Mott transition* merging to the fully ionized regime.

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**#P099 - Time-dependent optical systems and PT-Symmetric Hamiltonians**

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In recent years non-Hermitian Hamiltonian have been frequently used to describe dissipative effects in open optical systems. We consider a two-level atom interacting with a single cavity mode of the electromagnetic field in the rotating wave approximation, when one parameter of the system is periodically modulated in time. This system is also relevant for the dynamical Casimir and Casimir-Polder effects. In particular, we consider a periodically driven transition frequency of the two-level system and a periodic change of the frequency of the cavity mode. We show that, for appropriate choices of the system parameters, both cases can be simulated with a static non-Hermitian PT-symmetric JC Hamiltonian with an imaginary coupling constant. Finally, we investigate both mathematical and physical properties of this non-Hermitian Hamiltonian.

**#P100 - Halloysite as sustainable nanomaterial for water-in-oil emulsion stabilization**

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We prepared biocompatible hybrid halloysite nanotubes (HNTs) with a tunable hydrophobic/hydrophilic interface. The selective modification of the HNTs external surface with cationic surfactants endows to generate tubular nanostructures with an hydrophobic shell and an hydrophilic cavity. To this aim alkyltrimethylammonium bromides have been tested. The influence of the surfactants alkyl chain on the HNTs functionalization degree has been investigated. The dynamic behavior of the surfactant/HNT

hybrids in solvents with variable polarity has been correlated to their affinity towards hydrophobic media explored through partition experiments. Water contact angle experiments proved that lengthening the alkyl chain of the surfactant generates the enhancement of surface hydrophobicity. The water-in-oil emulsion is able to solubilize copper sulphate proving the incorporation and the loading of hydrophilic compounds into the HNTs lumen. Here we have fabricated eco-compatible reverse micelles with tunable hydrophobic/hydrophilic interface that might be suitable for industrial and biological applications as well as for selective organic synthesis. The prepared reverse inorganic micelles are efficient nanocontainers for the entrapment of the hydrophilic antibacterial agents. These features may be further exploited for biotechnological, conservation of cultural heritage and pharmaceutical applications.

#### #P101 - Tracking the molecular mouse trap mechanism in alpha1-antitrypsin with time-resolved X-ray solution scattering

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The inhibitory activity of proteins belonging to the serpin family is based on a peculiar mouse-trap mechanism: an exposed loop of the serpin molecule is cleaved by the target protease thus triggering the insertion of the loop into a beta-sheet of the serpin and the disruptive translocation of the protease. We have used time-resolved X-ray solution scattering to investigate the profound structural changes that occurs upon interaction of alpha1-antitrypsin (AAT), the prototypical member of the serpin family, and the protease chymotrypsin (CHY). Stopped-flow millisecond resolved experiments have been performed at the ID02 beamline of the European Synchrotron Radiation Facility (ESRF). The time evolution of the X-ray scattering patterns can be well described in terms of a kinetic model implying the presence of two distinct structural intermediates in the pathway connecting the Michaelis complex with the final stable AAT-CHY covalent complex.

#### #P102 - Inhibition of insulin aggregation by alpha-casein: the effect on different nucleation mechanisms as a tool for the investigation of amyloid formation

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The inhibition of protein aggregation is currently one of the most challenging topics in biomolecular research. Alpha-casein, which is abundantly found in bovine milk, has been recently shown to hinder the aggregation process in several proteins, including the amyloid beta-peptide, involved in Alzheimer disease<sup>1,2</sup>. The molecular mechanisms underlying this inhibitory effect are not completely clear and, given the importance and the multiplicity of the applications, need to be further investigated.

We studied the effects of alpha-Casein on insulin, a 51-residue hormone which constitutes a suitable model system for the investigation of the general properties of amyloid formation. Importantly, as for other proteins, insulin aggregation is known to be strongly affected by the existence of secondary nucleation pathways<sup>3-5</sup>. We show that alpha-casein has a very strong inhibiting effect on insulin amyloid formation, even at extremely low doses (down to 1:1000 molar ratio), when the aggregation process is characterized by secondary nucleation. At difference, the inhibitory effect is vanishing in other cases, such as the initial oligomer formation observed at high concentration, which does not involve secondary nucleation pathways<sup>6</sup>. These findings indicate that an efficient inhibition of amyloid formation can be achieved by chaperone-like systems by sequestering the early aggregates, before they become able to trigger the exponential proliferation brought about by secondary nucleation mechanisms. Moreover, the different extent of the chaperon-like activity of alpha-casein can help to single out the various steps and processes which affect amyloid formation.

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#### #P103 - COMPARISON OF CHARACTERISTICS OF FRICKE XYLENOL ORANGE GEL DOSIMETERS MADE WITH VARIOUS GEL MATRICES

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During the last decades, the interest in gel dosimeters for medical application has increased thanks to good properties that make them promising for good precision and high resolution measurements of the dose spatial distribution in radiotherapy. In particular, both Polymeric-gel and Fricke-XylenolOrange-gel (FXG) dosimeters were developed, but the FXG dosimeters possess further advantages for the application and have shown more reliable results.

It is known that FXG dosimeters have a dose response that depends on: i) the time elapsed between preparation and irradiation, ii) the time elapsed between irradiation and analysis, iii) subsequent irradiations. These characteristics result to be different for the different gelling agents. Various gel matrices have been investigated. Gelatin from porcine skin, Agarose and PVA are the gelling agents most commonly chosen for FGX dosimeters.

In this work, investigations have been carried out concerning the influence, on the dosimeter response, of the time elapsed between preparation and irradiation, or between irradiation and measurements. Moreover, the sensitivity of the dosimeters for subsequent exposures has been inspected. The results obtained with the three gelling agents, gelatin, Agarose and PVA, have been compared.

The achieved results have shown good consistency with the variation identified in the absorption spectra shapes for dosimeters irradiated with various doses and several subsequent exposures.

#### **#P104 - Dynamical weakening, remote triggering and acoustic fluidization in a fault system**

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The unexpected weakness of some faults has been attributed to the emergence of acoustic waves that promote failure by reducing the confining pressure through a mechanism known as acoustic fluidization, also proposed to explain earthquakes remote triggering. Here we validate this mechanism via the numerical investigation of a granular fault model system. We find that the stick-slip dynamics is affected only by perturbations applied at a characteristic frequency corresponding to oscillations normal to the fault, leading to gradual dynamical weakening as failure is approaching. Acoustic waves at the same frequency spontaneously emerge at the onset of failure in absence of perturbations, supporting the relevance of acoustic fluidization in earthquake triggering.

#### **#P105 - Time-of-flight analysers for Hard X-ray Photoelectron Spectroscopy at Free Electron Lasers**

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The advent of fourth generation synchrotron radiation facilities, namely the Free Electron Lasers (FELs), able to provide short (2 - 100 fs) but intense ( $10^{33}$  photons/s/mm<sup>2</sup>/mrad<sup>2</sup>/0.1%bandwidth) pulses of light also in the hard X-ray regime (photon energy above

2000 eV), opens new possibilities to study the ultrafast dynamics of processes exploiting the capability of Hard X-ray Photoelectron Spectroscopy (HAXPES) to measure core-level spectra of elements with bulk sensitivity.

In order to detect the intense bursts of high kinetic energy electrons generated by the X-ray pulses with an energy resolution comparable to that offered by the existing category of electron analysers, a new class of spectrometers also able to discriminate between electron bunches generated by consecutive photon pulses must be designed. A natural choice may be that of time-of-flight (TOF) spectrometers, which require a time reference in order to measure kinetic energies.

We present a characterisation of two different TOF spectrometers, namely one based on a standard retarding cylindrical lens and one based on the spherical reflector geometry<sup>1</sup>. SIMION® software has been used in order to evaluate electron trajectories of high kinetic energy electrons (5000 – 10000 eV) and extract transmission properties, angular acceptance and energy resolution. It resulted that while the linear system is able to accept a larger solid angle (cone aperture  $\pm 7^\circ$  for the linear TOF and  $\pm 2^\circ$  for the spherical reflector), the spherical mirror offers a better energy resolution (about 60 meV at 5000 eV kinetic energy compared to 1.5 eV at 10250 eV for the linear lens). This energy resolution values are obtained considering only the time resolution of the detector (such as a microchannel plate, MCP). Both analysers are capable to transmit a range of kinetic energies with a transmission above 90% wide enough to measure at the same time core level spectra from most elements (110 eV for the linear lens and 40 eV for the spherical reflector). Furthermore, we proved that both instruments are able to discriminate between two consecutive electron bunches having a temporal separation of about 220 ns as in the case of the European X-ray Free Electron Laser (XFEL), which is currently under construction at Hamburg.

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#### #P106 - Alanine/ESR dosimetry for electron Intra-Operative RadioTherapy: output factor measurements and Monte Carlo-GEANT4 simulations for IORT mobile dedicate accelerator

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Intra-operative radiation therapy (IORT) is a treatment modality where a single high dose of radiation is delivered directly to the tumor bed or to the exposed tumor during the surgical intervention, while avoiding surrounding dose-limiting structures. Mobile electron linear accelerators dedicated to IORT have been manufactured which have promoted a local large diffusion of this radiotherapy modality.

For breast irradiation, a single fraction of 21 Gy delivered on the target volume during the surgical procedure is equivalent to the total dosage (60 Gy) usually delivered during 30 external fractionated radiotherapy at 2Gy/fraction. Alternatively, a single dose of 10 Gy can be administered as Intra-Operative Boost to the tumor bed, followed by hypo-fractionated or conventional external beam whole breast radiotherapy.

This work reports a comparison between the response of alanine and Markus ionization chamber carried out for measurements of the output factors (OF) of electron beams produced by a linear accelerator used for IORT. Output factors (OF) for conventional high-energy electron beams are normally measured using ionization chamber according to international dosimetry protocols. However, the electron beams used in IORT have characteristics of dose per pulse, energy spectrum and angular distribution quite different from beams usually used in external radiotherapy, so the direct application of international dosimetry protocols may introduce additional uncertainties in dosimetric determinations. The high dose per pulse could lead to an inaccuracy in dose measurements with ionization chamber, due to overestimation of  $k_s$  recombination factor. Furthermore, the electron fields obtained with IORT-dedicated applicators have a wider energy spectrum and a wider angular distribution than the conventional fields, due to the presence of electrons scattered by the applicator's wall. For this reason, a dosimetric system should be characterized by a minimum dependence from the beam energy and from angle of incidence of electrons. This become particularly critical for small and bevelled applicators. All of these reasons lead to investigate the use of detectors different from the ionization chamber for measuring the OFs.

Furthermore, the complete characterization of the radiation field is achieved also by the use of Monte Carlo Geant4 simulations which allows to obtain detailed information on dose distributions. We compared the output factors obtained by means of alanine dosimeters and Markus ionization chamber. The results are characterized by a good agreement of response of alanine pellets and Markus ionization chamber and Monte Carlo results (within about 3%) for both flat and bevelled applicators.

#### #P107 - N-doped TiO<sub>2</sub> thin films photocatalytic applications

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Titanium dioxide (TiO<sub>2</sub>), thanks to its interesting properties as nontoxicity, low cost and high chemical stability, has been extensively investigated for several application in which, following light absorption, the generated charges can be usefully applied, as for photovoltaic applications or for photocatalytic devices. However, due to the wide intrinsic energy gap of TiO<sub>2</sub> (between 3.0 and 3.2 eV, depending on the crystalline structure), only a small fraction of the solar spectrum can be used to promote the light absorption. In the photocatalytic devices one of the most important goal of the recent research is to be able to prepare photocatalyst which can be active by absorbing the visible light, in order to increase the application of TiO<sub>2</sub>-based system in poor regions (where it could be difficult to use UV light sources) or to reduce the application cost. In order to increase the fraction of the solar spectrum that can be absorbed, different approaches have been used, mainly by doping TiO<sub>2</sub> with metals or anions.

In this paper we will present the results on the investigation on the photocatalytic properties of N-doped TiO<sub>2</sub> thin films deposited by drop-coating on different substrates (glass, alumina), both flat and as membranes. The solution was prepared using the sol-gel method and, after the deposition, the samples were annealed at different temperatures to promote the formation of a crystalline phase. The samples have been characterized by using X-ray photoemission spectroscopy (XPS), X-ray diffraction (XRD) and Secondary Electron Microscopy (SEM). The photocatalytic tests have been performed following the degradation of carbamazepine under illumination of visible light (from a solar simulator). The SEM images have shown the presence of a rough surface composed by nanocrystals, with an anatase form, determined by XRD, if the annealing temperature is higher than 300°C. The nitrogen concentration, determined by means of XPS, is quite low, about 2%, and decreases after the annealing process. From the careful analysis of the N1s peak, the presence of interstitial nitrogen has been reported. The photocatalytic tests have shown that the N-doped TiO<sub>2</sub> films are able to promote the degradation of carbamazepine up to about 70% of the initial concentration

#### #P108 - Anti-fibrillogenic effect of Hsp60 on A $\beta$ -peptide

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Alzheimer's Disease (AD) is the most common neurodegenerative disorder, whose incidence dramatically increases with the aging of the population. Signs and symptoms of clinically manifest AD are well characterized and one of the hallmarks of this devastating pathology is the formation of extracellular amyloid plaques in the brain. These deposits are composed by well-ordered,  $\beta$ -sheet rich, fibers of Amyloid  $\beta$  peptides (A $\beta$ ) produced by the aberrant proteolysis of the Amyloid Precursor Protein (APP) in residues of 39-43 amino acids. However, recent studies indicate that small soluble oligomers are more toxic than monomers or fibrils in causing neuronal disease. Based on this evidence, new therapeutic approaches mainly target the inhibition of A $\beta$  aggregation or deliver the unstable amiloidogenic monomers towards the formation of harmless and stable aggregates. In this context, molecular chaperones are crucial in targeting either the aggregation, or protein misfolding, or enhancing the clearance of toxic derivatives produced by A $\beta$ . Different chaperones have been already described as potential inhibitors of the fibrillation process of A $\beta$ . Indeed, these highly conserved cellular machines play a fundamental role in controlling protein misfolding and keeping the homeostasis in vivo throughout different and complex mechanisms. Compelling evidence by others and us indicates a mechanism of interaction between A $\beta$  and the mitochondrial chaperonin Hsp60 that might be crucial for the prevention of the neurological damage associated with AD pathology. However, the mechanism governing the A $\beta$ -Hsp60 interaction is not fully understood. In this work we investigate the role of Hsp60 in the aggregation pathway of A $\beta$  peptide. In order to achieve our goal, different biophysical techniques as fluorescence, circular dichroism spectroscopy, high performance liquid chromatography, atomic force microscopy (AFM) have been used. On the whole, our results indicate that the interaction between A $\beta$  and Hsp60 is characterized by an anti-amyloidogenic activity. Our results highlight the potential use of Hsp60 in the development of innovative strategies for AD treatment.

#### #P109 - Neuroserpin conformational disease: From molecular studies to therapeutic intervention

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Neuroserpin (NS) is a tissue plasminogen activator (tPA) serpin inhibitor in the brain, belonging to the SERPIN suprfamily and involved in different neurological pathologies, including the Familial Encephalopathy with Neuroserpin Inclusion Bodies (FENIB), related to the aberrant polymerization of neuroserpin mutants. So far, a pharmacological treatment of FENIB, i.e. an inhibitor of NS polymerisation, remains an unmet challenge. Here, we present the biophysical characterisation of the effects of embelin (EMB), a small natural compound, on NS conformational stability and polymerisation. EMB does not unfold NS molecules, but destabilises all known NS conformers, specifically binding to NS molecules. In particular, NS polymers disaggregate in the presence of EMB, and



their formation is prevented. The NS/EMB complex does not inhibit tPA proteolytic activity. Both effects are pharmacologically relevant: firstly by inhibiting the NS polymerisation associated to FENIB, and the secondly by antagonizing metastatic processes facilitated by NS activity in the brain.

#### #P110 - Characterization of skeletal muscle-derived extracellular vesicles (EVs): the effect of palmitoylation in EV biogenesis and the structural organization of their membrane

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Several cell types have the capacity to secrete extracellular vesicles (EVs) with a size ranging from hundreds to tens of nanometers (Exosomes), which contain cell-specific collections of proteins, lipids, and genetic material. Skeletal muscle (SkM) cells can release Alix-positive EVs (Romancino et al., FEBS J. 2013), suggesting a new paradigm for understanding how muscles communicate with other organs, such as adipose tissue, bones, the brain, or tumors. Here, we have used an integrated biological/biophysical approach to determine whether protein lipidation (*i.e.*, palmitoylation) affects the localization of EV modulator(s), EV biogenesis, and EV structural organization and heterogeneity. Protein palmitoylation was altered using a specific inhibitor (2-Br-Palmitate, 2BP). The biochemical analyses of exosome-specific biomarkers/regulators allowed us to determine that Alix is palmitoylated and that palmitoylation inhibition altered its subcellular localization. Also, we showed that palmitoylation inhibition altered the size and heterogeneity of EV, by using dynamic light scattering (DLS), that is here established as a routine technique to analyze and compare the size and diffusional properties of EVs in dispersion in different experimental settings. Small-angle X-ray scattering (SAXS) showed that the structural organization of the lipid bilayer of 2BP-treated EV, is qualitatively different compared to non-treated EV. Thus, we propose that palmitoylation might function to regulate the proper function of Alix in SkM-derived EV biogenesis and to maintain proper EV membrane structural organization. Beside its biological relevance, our study sets the route for a comprehensive structural characterization of EV, which is expected to be crucial in the design of engineered exosomes to be employed in the tissue regeneration field, *e.g.* to help in recovery from muscle atrophy and/or injury.

#### #P111 - Diffusion coefficient of PVA Fricke gel dosimeters

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Fricke gel dosimeters based on various matrix has been studied for a long time as 3D dosimetric system for radiotherapy. Self-oxidation and loss of spatial resolution due to diffusion have been the main issues that have impaired the affirmation of this technique so far. As part of an Italian nation-wide research program, we were interested in develop new gel formulations that are simple, reproducible and non toxic. We studied the one dimensional diffusion coefficient of Fe<sup>3+</sup> ions inside Fricke gel dosimeters based on a matrix of PVA cross-linked with a di-aldehyde. With a spectrophotometer equipped with a moving tray we were able to collect absorbance measurements at different positions of the gels. The method is simple, reproducible and has a good spatial resolution. We found that the amount of di-aldehyde influences the initial absorbance, as well as the cross-linking degree of the gel. We tested different compositions in order to combine a low initial absorbance, slow diffusion and a good sensibility.

#### #P112 - Patterns of high-frequency trading networks at NASDAQ OMX Helsinki

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We investigate trade networks and high-frequency sub-networks of market members trading at NASDAQ OMX Helsinki. We label a trade as a high-frequency trade if it belongs to a group of trades that are occurring with inter-trade time intervals shorter or equal to one millisecond. For several securities we monthly analyze the networks of high-frequency trades between pairs of market members. We perform a statistical validation [1] of the links forming these networks against a random null hypothesis which preserves the heterogeneity of each market member's performed transactions. The statistically filtered networks, containing both over-expressed and under-expressed links, allow the identification of actual high-frequency trading players and market members who are trading by them. We also provide statistical evidence of the presence of preferential relationships between market members in the network consisting of all trades for a given security, in spite of market anonymity. A possible correlation between the validated network of all trades and the validated network of high-frequency trade is examined.

[1] Tumminello M, Miccichè S, Lillo F, Piilo J, Mantegna RN (2011) Statistically Validated Networks in Bipartite Complex Systems. PLoS ONE 6(3): e17994. doi:10.1371/journal.pone.0017994

**#P113 - Dosimetry to Electron Spin Resonance (ESR) using organic compounds (alanine and ammonium tartrate) for mixed neutron-gamma fields**

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Alongside with the development of Neutron Capture Therapy (NCT) and the use of thermal neutrons for radiotherapeutic purposes, many efforts have been devoted to the characterization of the beam in order to optimize therapy procedures. Reliable dose measurements should be able to determine the various (neutrons and photonic) components of the mixed beam usually employed for therapy.

This paper studies the effect of additives such as Boric and Gadolinium nuclei on the sensitivity of neutron organic (alanine and ammonium tartrate) dosimeters analyzed through Electron Spin Resonance (ESR) technique. These dosimeters were exposed to a mixed (neutron-gamma) field mainly composed of thermal neutrons. The choice of  $^{10}\text{B}$  and  $^{64}\text{Gd}$  as nuclei additives is due to their very high capture cross section for thermal neutrons. Also, after the nuclear reaction with thermal neutrons are emitted particles, which in turn release their energy in the vicinity of the reaction site.

The irradiation with mixed (neutron-gamma) field were performed within the thermal column of the TRIGA reactor, University of Pavia. Dosimeters readout was performed through the Electron Spin Resonance (ESR) spectrometer Bruker ECS106 located at the Laboratory of Dosimetry ESR / TL of the Department of Physics and Chemistry - University of Palermo.

We found that the addition of Gadolinium allows to largely increase the sensitivity of the dosimeters for thermal neutrons. In particular, a low concentration (5% by weight) of gadolinium oxide leads to an improvement of the sensitivity of neutrons more than 10 times. In addition, for this low content of gadolinium the photon tissue equivalence is not heavily reduced. This experimental analyses are compared with computational analyses carried out by means of Monte Carlo simulations performed with the MCNP (Monte Carlo N-Particle) transport code. A good agreement was observed for alanine dosimeters.

**#P114 - Agarose and PVA Fricke gel dosimeters exposed to clinical photons beams: Nuclear Magnetic Resonance Relaxometry and Imaging**

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Fricke Xylenol Gel (FXG) dosimetric system is based on the radiation induced oxidation of ferrous ( $\text{Fe}^{2+}$ ) to ferric ( $\text{Fe}^{3+}$ ) ions.

The application of Fricke gels for ionizing radiation dosimetry is continuously increasing worldwide due to their many favorable properties. However, one of their shortcomings is that ferrous and ferric ions diffuse in the gel matrix. To maintain the spatial integrity of the dose distribution, Fricke gels must be undergoing measurement within a few hours of their irradiation, so that ferric ions remain close to their point of production. Thus, the spatial integrity of the dose distribution in the Fricke gel is maintained.

The gel matrix also contributes to the oxidation of ferrous ions during irradiation, increasing the chemical yield of ferric ions in aqueous solution and increasing the sensitivity of the dosimeter.

The oxidation of ferrous ions also causes a reduction of the longitudinal nuclear magnetic relaxation time  $T_1$  which can be measured by means of Nuclear Magnetic Resonance Relaxometry (NMR) and Magnetic Resonance Imaging (MRI).

The results presented are related to an experimental investigation conducted on Fricke Gels characterized by gelatinous matrix of Agarose or PVA.

We performed NMR relaxometry investigations which allow for direct measurements of the relaxation times in samples exposed to clinical photon beams. The main dosimetric features of the NMR signal were investigated. The gels were irradiated in the clinical dose range between 0 and 20 Gy. In order to assess the photon sensitivity we analyzed the dependence of NMR relaxation time on radiation dose with varying ferrous ammonium sulfate content inside FXGs. Furthermore, signal stability was followed for several days after irradiation.

These measurements were preliminary to MRI analysis which can permit 3D dose mapping. In order to optimized the MRI response a systematic study was performed to optimize acquisition sequences and parameters. In particular, we analyzed for inversion recovery sequences the dependence of MRI signal on the repetition time  $T_R$  and on the inversion time  $T_I$ .

The dose calibration curves are reported and discussed from the point of view of the dosimeter use in clinical radiotherapy. This work has highlighted that the optimization of additives inside gel matrix is fundamental for optimizing photon sensitivity of these

detectors. We can conclude that FXG dosimeters with optimal ferrous ammonium sulfate content can be regarded as a valuable dosimetric tool to achieve fast information on spatial dose distribution.

### #P115 - Functional oxides for nano-electronics and spintronics

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Complex transition metal oxides present interesting physical phenomena, such as high dielectric permittivities, ferroelectricity and multiferroicity. Their extreme sensitivity to structural distortions and crystal chemistry offers many routes to control these properties. Here we report our activity on multiferroic and high-k oxides.

BiFeO<sub>3</sub> (BFO) is a promising multiferroic material for its high ordering temperatures far above room temperature (Néel temperature  $T_N = 643\text{K}$  and a ferroelectric ordering below  $T_C = 1103\text{K}$ ). A robust and large exchange bias effect has been demonstrated at room temperature in BiFeO<sub>3</sub>/CoFeB heterostructures. The exchange bias and magnetoelectric coupling at a BFO/ferromagnet interface can play a key role in the development of electrically controlled spin devices. Our activity ranges from target preparation and optimization to a systematic study of thin films deposited by PLD. The realization of targets with phase and stoichiometry control still represents a significant task, since the quality of the BFO film strongly depends from target characteristics. Structural, dielectric and ferroelectric characterizations of both bulk and thin films were performed using X-Ray Diffraction, impedance spectroscopy and ferroelectric characterization by means of a train pulses technique, named PUND (positive-up negative-down), and piezoresponse force microscopy (PFM). A systematic study was then performed to understand the role of each deposition parameter, such as substrate temperature, oxygen pressure on the structure and impure phase formation during BFO film growth. It was found that a non-stoichiometric target is preferable to limit the effect of bismuth losses and contain the impure phase formation. Increasing the oxygen pressure, improved dielectric properties have been observed, due to the decreasing number of oxygen vacancies.

Bulk Y<sub>2</sub>CuTiO<sub>6</sub> (YCTO) showed high dielectric constant ( $\epsilon'$ ) and very small dielectric loss. In resonators, antennas and transmitters, a high dielectric constant and a low dielectric loss are important to miniaturize the devices and reduce the bandwidth. Moreover, novel materials with improved dielectric properties are required to enhance the performance of CMOS field-effect transistors and to allow further miniaturization. However a quantitative analysis of the thin films is necessary for device applications. In our work we compared the dielectric properties of YCTO thin films prepared by PLD and characterized for their dielectric properties in comparison with SiO<sub>2</sub> and MgO. The dielectric constant of YCTO thin films was found to vary from 22 up to 100 at 100 kHz for the films deposited at 0.5 and 0.05 Pa oxygen pressure, respectively. This last value is about 25 times higher than for SiO<sub>2</sub> and 10 times higher than MgO.

Work to implement these materials in electronic and spintronic devices is currently in progress.

### #P116 - Nanocomposite based on Multi-Macrocyclic Receptors and Halloysite for Volatile Organic Compounds Capture

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Volatile organic compounds (VOCs) are chemicals released to the atmosphere by natural and anthropogenic sources. VOCs are hazardous air pollutants and promote formation of photochemical smog. Variety of chemicals released from pharmaceutical industry includes priority pollutants like benzene, toluene, and dichloromethane. The aim of this work was at designing, preparing and characterizing from the physico-chemical view-point a pseudo nano-sponge with low environmental impact for pollutant removal. As adsorbent material, a nanocomposite based on nanoclay and cucurbiturils, which are biocompatible materials, were investigated.

Clay minerals (e.g. montmorillonite and kaolin) are important components of soils and sediments. Many have strong sorption affinities, large specific surface areas and high cation exchange capacities. These aluminosilicates have been tested since more than 40 years ago in the removal of toxic metals or organic pollutants. Among the aluminosilicates, halloysite (Al<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub>·nH<sub>2</sub>O) is a special nano-geomaterial because of its tubular morphology, high porosity and tunable surface chemistry which enabled it to be utilized as a promising adsorbent for various organic pollutants.

Cucurbiturils are cyclic polymers of glycourils which can exhibit similar host-guest chemistry as cyclodextrins. There are different homologues of cucurbiturils among which CB[8] selected in this work can hold small gas molecules, aliphatic and aromatic guests. The adsorption capability of hybrid nano-sponge was investigated and correlated to the structural feature of the adsorbent sustainable nanomaterial. Toluene was selected as contaminant prototype.

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**#P117 - Laser assisted atomic ionization by a short XUV pulse**

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We report on numerical results of energy spectra of photoelectrons emitted by irradiating an hydrogen atom with a relatively weak single attosecond XUV pulse in the presence of a two-color IR laser pulse. The densities of probabilities have been obtained by treating the interaction of the atom with the XUV radiation at the first order of the time-dependent perturbation theory and describing the emitted electron through the Coulomb-Volkov wavefunction. The results of the calculations agree with the ones found by numerically solving the time-dependent Schrödinger equation. Specifically, we use an algorithm that implements an high precision variant of the Crank Nicolson integration method and allows to take into account the singularity in the Coulomb potential. Analysis of the spectra obtained for very long pulses show that certain features may be explained in terms of quantum interferences in the time domain.

**#P118 - High-order harmonic generation via bound-bound transitions in elliptically polarized laser field**

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We use a 5-level system to investigate the HHG spectrum emitted by an atom driven by a linearly or elliptically polarized laser field. For this model the Schrodinger equation is numerically solved and we study the dipendence of the spectra, harmonic intensity and polarization of emitted radiation on the laser field ellipticity. Studying the intensity of the emitted radiation we find that un alsoder high laser ellipticity the harmonic emission is greatly reduced; the analysis of results shows that the harmonic intensity and the emitted radiation depend on the laser ellipticity.

**#P119 - Dynamical Properties of the Homogeneous Electron Gas from Auxiliary Fields Quantum Monte Carlo**

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Quantum Monte Carlo (QMC) simulations of many body fermionic systems are considerably complicated by the well known sign problem [1]. Although very accurate approximation schemes have been developed for the calculation of static properties, the possibility of extending such methodologies to the investigation of dynamical properties is still largely unexplored [2]. Recently, a number of innovative QMC methods have been conceived, which map the imaginary time evolution into a random walk in the manifold of Slater determinants. In such methods the sign problem emerges in a different form, and can be treated introducing approximations that are more likely to permit the study of excited states [5]. We have focused on the phaseless auxiliary Fields QMC method (AFQMC), developed by S. Zhang [3]. Generalizing the formal manipulations suggested by F. Assaad et al. [4], we propose a practical scheme to evaluate dynamic correlation functions in imaginary time, giving access to the response functions of interacting fermionic systems. We assess the accuracy of the methodology via the study of exactly solvable simple models, comparing AFQMC predictions with exact solutions [5]. We also compute the imaginary time correlation functions and the effective mass of the two-dimensional homogeneous electron gas in the high-density regime, providing comparison between AFQMC results and other QMC methods, and with recent experimental data [6].

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**#P120 - Scaling behaviours at first order quantum transitions**

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The theoretical description of phase transitions and critical phenomena primarily takes place in the ideal settings of infinite and spatially homogeneous conditions. Yet the way in which a system undergoes a phase transition can be substantially modified by its

finiteness and the presence of inhomogeneities. At continuous phase transitions, characterised by the development of diverging correlations at criticality, the theories of finite-size scaling (FSS) and trap-size scaling (TSS) can account for the modified critical behaviours of systems in finite and inhomogeneous conditions, respectively.

Systems that undergo first-order (or discontinuous) phase transitions are characterised by discontinuities of thermodynamic quantities across the transition and do not develop diverging correlations at the transition in the thermodynamic limit. Nevertheless, finite-size effects do affect these systems, in the form of a rounding and smoothing of the transitions' discontinuities. After reviewing our understanding of scaling behaviours at continuous transitions, we show that sensible theories of FSS and TSS can be put forward in the context of finite or inhomogeneous systems undergoing first order quantum transitions (FOQT). Our results are confirmed by numerical simulations on the quantum Ising chain in transverse and parallel fields and on the q-state quantum Potts chain with  $q > 4$ , both affected by FOQT. Our theory is especially important in the interpretation of experimental or numerical data, providing tools to discriminate between a smoothed discontinuous transition and a genuine continuous transition.

### #P121 - Functional connectivity modulation induced by transcranial direct current stimulation of the motor network investigated by resting state fMRI

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During rest the brain network is not idle, but rather shows a vast amount of spontaneous activity that is highly correlated between multiple brain regions. Resting state functional Magnetic Resonance Imaging (rs-fMRI) analyses focuses on spontaneous low frequency fluctuations ( $< 0.1$  Hz) in the BOLD signal and investigates synchronous activations between regions that are spatially distinct (functional connectivity, FC), occurring in the absence of a task or stimulus.

Transcranial Direct Current Stimulation (tDCS) is a non-invasive brain stimulation technique that is known to modulate cortical activity and FC among brain regions, as measured by functional Magnetic Resonance Imaging. It is well established that motor response (motor evoked potentials, MEP) is enhanced by anodal tDCS stimulation and reduced after cathodal tDCS stimulation, for a period of about 5 minutes. Further studies showed different patterns of FC modulation after tDCS, depending on polarity but also on the regions studied, but little is known about the duration of the effect.

This study is aimed at measuring the variation of functional connectivity between cortical brain regions after tDCS along time. For this purpose we enrolled 20 healthy right-handed subjects. All subjects underwent 4 sessions RS-fMRI (10' each, TR 2'', 300 volumes, 1.5T scanner): 2 immediately before and 2 after 20' tDCS over left M1. 12 of them received real (anodal) tDCS, 8 received sham stimulation. Data from 6 subjects (5 real, 1 sham) have been excluded for movement artifacts or other technical problems. We analyzed FC between left and right M1 with two different statistical analyses: *Seed-based Correlation Analysis* (SCA) and the *Temporal Concatenation Group ICA* (TC-GICA).

Seed-based Correlation Analysis showed a significant decrease of FC during the first fMRI acquisition immediately after anodal tDCS stimulation ( $p=0.005$ ), that got back to baseline during the last fMRI session. This behavior was not found in subjects who underwent sham stimulation ( $p=0.12$ ).

The *Temporal Concatenation Group ICA* (TC-GICA) showed that immediately after anodal stimulation the average value of voxels decreases significantly ( $p < 0.05$ ) whereas there is no significant decrease in the case of sham tDCS stimulation.

Our results shows that anodal tDCS is able to induce connectivity changes within motor network, that is reversible in a period lasting between 10' and 20' after stimulation.

### #P122 - A fourth-order method for the calculation of Casimir-Polder forces in terms of vacuum fluctuations and radiation reaction field

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We consider two two-level atoms interacting with the relativistic scalar field in the vacuum state or in a thermal state. We extend to the fourth order in the coupling constant the general procedure by Dalibard, Dupont-Roc and Cohen-Tannoudji [1], in order to evaluate the dispersion interaction energy between the atoms and separate it in contributions from vacuum fluctuations and radiation reaction field. This method can be also easily generalized to the electromagnetic field and to other states of the field. By considering the rate of change of an arbitrary atomic observable  $G_{A/B}$  given by the Heisenberg equations (A and B indicate the two atoms), we exploit the possibility to split the field and atomic operators in a free and a source part. We thus obtain two different contributions to the evolution rate of  $G_{A/B}$  with a clear physical origin: a *vacuum fluctuations* contribution that can be interpreted as due to field fluctuations inducing correlated polarizations on the two atoms,

and a *radiation reaction* contribution due to the presence of the atoms that polarize the field which in turn reacts back on the atoms. Our method is pretty general and the equations obtained for the fourth-order interaction energy can be also used in several physical situations. In particular, we apply it to evaluate the dispersion interaction energy between the two atoms in three different cases: atoms at rest in the vacuum, atoms at rest in a thermal bath and atoms accelerating in the same direction in the vacuum [2]. The latter case is also related to the Unruh effect.

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#### **#P123 - The influence of interparticle correlations on the scattering and birefringence in magnetic fluids: combined simulation and theoretical study**

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Commercial magnetic fluids are polydisperse stable suspensions of single domain magnetic particles. Ferroparticles of such small sizes (typical diameter 10–20 nm) can be considered as uniformly magnetized; each particle has a permanent magnetic dipole moment. The magnetic cores are usually stabilized with a surfactant shells to prevent particle agglomeration. In theory one usually employs dipolar hard sphere model to describe the properties of ferrofluids. Another efficient method to describe the response of magnetic fluids is to use a computer simulations. We choose bidisperse system as the first step to take into account polydispersity of ferrofluids when studying thermodynamics of magnetic fluids. Using molecular dynamics simulations, we calculated polydisperse structure factor and compared it to a model bidisperse structure factor calculated analytically. It is well-known that magnetic fluids when subjected to an external magnetic field exhibit birefringence. We check the analytical model for a bidisperse system with chains by comparing to the results of computer simulations for the dipolar system with multiple fractions. From this two approaches we conclude: the bidisperse approximation based on matching the magnetic properties is not always appropriate for the description of the scattering properties of polydisperse dipolar systems, whereas this model can provide satisfactory results for birefringence.

#### **#P124 - Conformational Dependence of the Circular Dichroism Spectra of Single Amino Acids from Plane-Waves-Based Density Functional Theory Calculations**

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We study the conformational dependence of circular dichroism (CD) spectra of amino acid molecules by means of an efficient ab initio DFT approach which is free from the typical gauge invariance issues arising with the use of localized basis sets and/or real-space grids. We analyze the dependence of the chiroptical spectra on the backbone dihedrals in the specific case of alanine and consider the role of side chain degrees of freedom at the examples of leucine, phenylalanine, and serine, whose side chains have different physicochemical properties. The results allow one to identify the most diagnostic regions of the CD spectra and to critically compare the conformations which match the experimental CD data with conformations extracted from the rotamer library. The inclusion of a solvation shell of explicit water molecules and its effect on the CD spectrum are analyzed at the example of alanine.

#### **#P125 - Carbon sp wires coupled to graphitic fragments: stability, electronic properties, and oxidation effects.**

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Nanostructured carbon containing monoatomic linear chains is a paradigmatic example of a system where the interplay between electronic properties and structural degrees of freedom lead to many exciting potential applications, ranging from nanoelectronics to spintronics [1]. We show how mechanical, electronic, vibrational and magnetic properties of systems containing  $sp$  monoatomic wires coupled to  $sp^2$  graphitic fragments are influenced by structural details, such as the geometry of chain terminations or tensile and torsional strain. DFT theoretical results suggest that  $sp$ -carbon chains are strongly stabilized by bonding to the edges of graphitic nanofragments, a results which has subsequently be confirmed by many experimental findings. Quantum electron conductances exhibit narrow resonant states resulting from the simultaneous presence of open conductance channels in the contact region and on the chain atoms, so that the system behaves as a spin-polarized semiconductor. The calculation of vibrational properties within Density Functional Perturbation Theory allow us to interpret the nontrivial features of experimental Infrared and Raman spectra of cluster-beam deposited pure-carbon samples, including the spectral modifications and decay induced by exposure to air [2-5], with infrared spectra probing the effects of oxidation on  $sp$ - and on  $sp^2$ -hybridized carbon separately.

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#### #P126 - Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against GW band structure calculations and experiments

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We investigate band gaps, equilibrium structures, and phase stabilities of several bulk polymorphs of wide-gap oxide semiconductors  $ZnO$ ,  $TiO_2$ ,  $ZrO_2$ , and  $WO_3$ . We are particularly concerned with assessing the performance of hybrid functionals built with the fraction of Hartree-Fock exact exchange obtained from the computed electronic dielectric constant of the material. We provide comparison with more standard density-functional theory and GW methods. We finally analyze the chemical reduction of  $TiO_2$  into  $Ti_2O_3$ , involving a change in oxide stoichiometry. We show that the dielectric-dependent hybrid functional is generally good at reproducing both ground-state (lattice constants, phase stability sequences, and reaction energies) and excited-state (photoemission gaps) properties within a single, fully ab initio framework.

#### #P127 - Atomistic study of the structural and electronic properties of a-Si:H/c-Si interfaces

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We investigate the structural and electronic properties of the interface between hydrogenated amorphous silicon (a-Si:H) and crystalline silicon (c-Si) by combining tight-binding molecular dynamics and DFT ab initio electronic structure calculations. We focus on the c-Si(100)(1×1)/a-Si:H, c-Si(100)(2×1)/a-Si:H and the c-Si(111)/a-Si:H interfaces due to their technological relevance. The analysis of atomic rearrangements induced at the interface by the interaction between H and Si allowed us to identify the relevant steps that lead to the transformation from c-Si(100)(1×1)/a-Si:H to c-Si(100)(2×1)/a-Si:H. The interface electronic structure is found to be characterized by spatially localized mid-gap states. Through them we have identified the relevant atomic structures responsible for the interface defect states, namely: dangling-bonds, H bridges, and strained bonds. Our analysis contributes to a better understanding of the role of such defects in c-Si/a-Si:H interfaces.

#### #P128 - Multiphoton k-resolved photoemission from gold surface states with 800-nm femtosecond laser pulses

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We measure direct multiphoton photoemission of the Au(111) surface state with 800-nm laser pulses. We observe the parabolic dispersion in the angular distribution of photoelectrons having absorbed between four and seven photons. The k dispersion we measure can be explained in terms of Shockley-state replicas, with a nascent hot electrons distribution at k above the Fermi level. Moderate laser power densities, of the order of  $100\text{GW}/\text{cm}^2$ , resulted in large electron yields, indicating the importance of multiphoton excitations to define the electronic and magnetic properties of matter in the first hundred femtoseconds after laser excitation.

#### #P129 - Multiphoton k -resolved photoemission from gold surface states with 800-nm femtosecond laser pulses

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We measure direct multiphoton photoemission of the Au(111) surface state with 800-nm laser pulses. We observe the parabolic dispersion in the angular distribution of photoelectrons having absorbed between four and seven photons. The k dispersion we measure can be explained in terms of Shockley-state replicas, with a nascent hot electrons distribution at k above the Fermi level. Moderate laser power densities, of the order of  $100\text{GW}/\text{cm}^2$ , resulted in large electron yields, indicating the importance of multiphoton excitations to define the electronic and magnetic properties of matter in the first hundred femtoseconds after laser excitation.

#### #P130 - ESPI non-destructive testing of composite materials for aeronautical application

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In this study, ESPI technique has been used to evaluate the effective delaminated area of damaged Epoxy-Carbon Fibers and Glass Fibers composites. The analyzed specimens have been manufactured by a vacuum assisted infusion process. In order to obtain the composite panels, a one-component commercial aeronautical resin (RTM6 from Hexcel) was used with eight dry unidirectional carbon or glass plies having a quasi-isotropic stacking sequence  $[0^\circ, 90^\circ, +45^\circ, -45^\circ]$ . The obtained panels have been subjected to low velocity impact tests at different impact energy levels (i.e. 6, 10, 13J) or flexural tests according with the ASTM D790 standard. The panels were afterwards analyzed by means of ESPI. Through real-time surface illumination by visible laser (i.e. 532 nm), where range and accuracy are related to the wavelength and the deformation value is measured by half-wavelength laser multiples, the ESPI technique allowed the non-contact, non-destructive detection of micro-deformations, micro-cracks, residual stress and delamination usually non detectable by visual inspection. A CCD camera records the whole field image of the surface differential displacement caused by a non-destructive thermal or mechanical deformation. By this technique and with suitable image processing, it is possible to reveal hidden defects. In composite laminates, the delamination occurs on the opposite side of the impact face and it is not visible under the barely visible threshold so, thanks to ESPI it is possible to reveal the presence of the damage and to evaluate the effective delaminated area. A good agreement between the experimental results and literature has been found confirming the reliability of the proposed technique.

#### #P131 - Oxygen sensing of mixed-phase titanium dioxide nanostructures

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Oxygen-detecting properties of titanium dioxide ( $\text{TiO}_2$ ) are investigated by continuous wave photoluminescence (CWPL) and photoluminescence excitation (PLE) spectroscopy. An interesting double modulation in the photoluminescence due to adsorption of oxygen is evidenced in differently structured samples, from sintered nanopowders to highly porous hierarchical quasi-1D nanostructures, when two  $\text{TiO}_2$  crystal phases are mixed. Surface interaction with  $\text{O}_2$ , in fact, produces opposite responses in rutile and anatase photoluminescence efficiency. This feature can open a promising path in the optical gas sensing branch. Moreover, a broad range investigation allowed us to clarify the mechanisms at the origin of PL emission in  $\text{TiO}_2$ , that are found to involve different electronic states as initiators in addition to the standard Schottky barrier mechanism commonly accepted in most metal-oxide sensors. Our findings pointed out the potentialities for future double-parametric optical sensing by titania thanks to multiple response obtained from a same analyte, and possibly paved the way for selective detection towards chemical species carried in air.



**#P132 - Investigation of applicability of alanine pellets and films for dosimetry of proton clinical beams**

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Laser-driven proton has recently gained a great interest as an alternative to conventional and more expensive acceleration techniques. These ion beams have desirable qualities such as small source size, high luminosity and small emittance to be used in different physics fields. This is very promising specially for the future perspective of a new concept of hadrontherapy based on laser-based devices could be developed, replacing traditional accelerating machines.

ELIMED (Medical Applications at Extreme Light Infrastructure) is a task-force originally born by an idea of ELI-Beams (Prague) and INFN-LNS (Italian Institute for Nuclear Physics of Catania) researchers.

ELIMED main goal is to perform proof-of-principle experiments aimed to demonstrate that laser-accelerated high-energy proton beams (up to 70 MeV in the first phase) can be potentially used for the specific case of ocular proton therapy.

In this work we report the investigation of the dosimetric features of alanine pellets exposed to protons produced by means of the CATANA (Centro di AdroTerapia e Applicazioni Nucleari Avanzate) proton therapy facility. This analysis is preliminary for the application of the alanine dosimeters in laser-driven proton beams.

ESR spectrometry with alanine is now widely recognized as the most accurate method of transfer dosimetry in the industrial (kGy) dose range. It is well established for calibrating industrial radiation sources against national standards (NIST, IAEA, NPL) and for comparisons between national laboratories. The accuracy of the method is generally very high, largely due to the low sensitivity of the alanine response to irradiation variables (energy, dose rate, temperature, etc.), and the ability of ESR spectrometers to measure dosimeter signals very precisely. As a matter of fact, the main requirements for a suitable system such as: linear response to dose, sensitivity, tissue equivalence, absence of energy dependence, absence of fading, small dimensions, ruggedness, and non-destructive readout, to a large extent are met by the alanine/ESR dosimetry.

Here we analyzed the performances of two different alanine/ESR systems (3 mm pellets and 0.1 mm films) irradiated with therapy proton beams (62 MeV). The LET dependence of the response was obtained from the analysis of pellet irradiated with a modulated beam. The energy dependence of the response was derived from the analysis of film stacks irradiated with pristine beams. Use of thin films allowed for a high resolution sampling of the proton slowing down mechanisms. Alanine measurements are compared with Markus parallel plate ionization chamber and are aided by Monte Carlo calculations for medical physics using GEANT4 code.

**#P133 - Comparison of EPR response of pure alanine and alanine with gadolinium dosimeters exposed to TRIGA Mainz reactor**

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The development of Neutron Capture Therapy (NCT) for cancer treatments has stimulated the research for beam characterization in order to optimize the therapy procedures. The NCT has found to be promising for treatments of tumours which hardly can be treated with other techniques, such as gliomas. Alongside with the improvements of this technique, the development of procedures for the beam characterization arouses great interest in order to optimize the therapy protocol by reliably determining the various (neutronic and photonic) components of the mixed beam usually employed for therapy.

Electron Paramagnetic Resonance (EPR) dosimetry for electron and photon beams with alanine has attracted the attention of many research groups for dosimetric purposes. Furthermore, the applications of EPR dosimetry for high LET radiation beams, such as carbon ions and neutrons, are continuously increasing. This is because of the very good dosimetric features of alanine EPR detectors such as: tissue equivalence for photon beams, linearity of its dose-response over a wide range, high stability of radiation induced free radicals, no destructive read-out procedure, no need of sample treatment before EPR signal measurement and low cost of the dosimeters. Moreover, in order to improve the sensitivity to thermal neutrons of alanine dosimeters the addition of nuclei such as gadolinium oxidewas previously studied.

The choice of Gd as additive nucleus is due to its very high capture cross section to thermal neutrons and to the possibility for secondary particles produced after interaction with thermal neutrons of releasing their energy in the neighbourhood of the reaction site. In particular, it was found that low concentration (i.e. 5% by weight) of gadolinium oxide brings about a neutron sensitivity enhancement of more than 10 times without heavily reducing tissue equivalence.

We have studied the response of alanine pellets with and without gadolinium exposed to the thermal column of the TRIGA Mark II research reactor at the University of Mainz.

Pure alanine dosimeters used were produced by Synergy Health (Germany) whereas the Gd-added dosimeters were produced at the University of Palermo. The irradiations were performed inside polyethylene holders to guarantee charged particles equilibrium conditions.

The results of EPR experiments are compared to Monte Carlo (MC) simulations aimed at obtaining information about the contribution of the various components to the total dose measured by means of EPR dosimeters. For alanine dosimeters a good agreement between experimental data and MC simulation have been achieved.

#### #P134 - Self-healing of epoxy composites using resin/hardener containers

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Self-healing polymer composites have been an intense field of research for the past decade. These materials have the inherent ability to heal damage event either autonomically or nonautonomically with external intervention (heat, light and etc.). For the past years, different types of healing systems are being proposed which include capsule-based, vascular-based and intrinsic self-healing systems. Under capsule-based self-healing system, dual capsule healing mechanism shows promising results due to its simple healing mechanism and cost effectiveness. This healing system comprises of monomer and polymeriser/hardener which are being encapsulated separately and embedded into polymer matrix homogeneously. As internal cracks emerged and rupture these capsules, the liquid monomer and polymeriser will be released into the crack plane, polymerised and eventually heal the crack. However, there are underlying limitations for this self-healing mechanism such as one time healing cycle, cruciality of monomer and hardener stoichiometric ratio for addition polymerisation healing chemistry. Thus, the dispersion homogeneity is essential for complete healing. Besides, the difficulties in encapsulating reactive nature hardeners is also one of the limitation. For two-part epoxy system, mixing and breaking both carrier networks is a challenge. There are two objectives in this study. First, to design and fabricate a dual capsule self-healing polymer composite with multiple healing cycles without compromising the mechanical properties of the polymer composite itself. Subsequently, using electrospun nanofibrous mats of polyacrylonitrile (PAN) carrying epoxy and amine dual healing solutions into an epoxy matrix to impart self-healing functionality. The self-healing performance of the epoxy composites was measured using fracture toughness tests. The average healing efficiency was approximately 75% at 50C and 38% at room temperature. The epoxy composites were capable of repeated self-healing for up to 6 times at room temperature. These new methods of preparing self-healing epoxy is cheap and versatile and can be optimized for mass production of high performance self-healing structural composites.

#### #P135 - Nanomechanical characterizations by atomic force microscopy

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Advancement in nanoscience and nanotechnology is strongly related to that in nanometrology and to the development of techniques for the investigation of physical and chemical properties of materials at the nanometer scale. In particular, methodologies for a mechanical characterization of materials in a wide range of Young's moduli are required, from stiff to compliant materials including biological samples.

Atomic force microscopy (AFM) represents a powerful technique for the development of mechanical single-point measurements and imaging techniques with lateral resolution in the nanometer scale, due to its unique capabilities of scanning the surface at a nanometer resolution in combination with the possibility of exerting ultra-low loads on the sample surface.

Here, we review three AFM based techniques for the accurate measurements of mechanical properties of either stiff or compliant materials at a nanometer scale. Contact resonance AFM (CR-AFM), AFM-based depth sensing indentation (AFM-DSI), and torsional harmonics AFM (TH-AFM) are briefly described. The ranges of Young's modulus values in which they can be used (overall, from a few hundreds of gigapascals to a few tens of megapascals) and the different penetration depths (which permits the investigation of both bulk and near surface mechanical properties) are discussed. The reported examples of application of these techniques include gemstones and minerals, diamond-like carbon coatings, ultrathin films, polymeric materials (films, blends, fibers and nanofibers) also reinforced with nanodiamond particles, biological samples as collagen fibers or cells internalizing stiff nanoparticles.

#### #P136 - Biosensing with silicon photonics

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Silicon photonics allows integrating photonic components in silicon with high integration density and high functional performances. In this talk, I will present few applications where biosensing is performed by using silicon photonic devices. The first example will be an evanescent field based luminescent biosensors where waveguides are used to channel light into an integrated bioreactor where a fluorescent probe is covalently immobilized and detected, as proof of principle for protein detection through fluorescence(1). The second example is based on porous silicon membranes which act as flow through polarimetric sensors to detect allergens in food (2). The last example is about label free whispering gallery mode biosensors where functionalized label-free microresonators are able to sense the presence of aflatoxins in milk (3).

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(1)Journal of Physics D: Applied Physics 47, 405401 (2014).

(2)Optics Express 19, 26106 (2011).

(3)Sensors (2015) [arXiv:1408.3954]

### #P137 - Electronic properties of molecular Fe complexes deposited on Graphene/Ni(111)

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Transition metal complexes adsorption on surfaces is an important issue in fundamental physical science, and is also significant for various applications in new industries. Interconnection between electronic and magnetic properties of these complexes is a crucial issue in this field and a fine characterization of the interface electronic properties is mandatory. Recent results of phthalocyanines deposited on ferromagnetic metallic surfaces and graphene buffer layers have revealed a substrate-molecular coupling mechanism. In case of elemental transition metals adsorbed on graphene electronic- structural changes of the metal layers have shown a delicate interplay between long-range interactions and local chemical bonding, influencing the adatom equilibrium distance and magnetic moment. In this work a combination of NEXAFS and X-ray photoelectron spectroscopy have been employed to study the adsorption of Fe-complexes molecules, (ferrocene, Fe(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub> and tetraphenyl Fe-Cl porphyrin (FeTPP-Cl) deposited on well characterized graphene supported by Ni(111) and compared with adsorption on HOPG substrate. The two set of molecules have been chosen for their different structural surrounding of the Fe ion and the different distance between Fe atom of adsorbed molecules and the substrate. Physisorbed Ferrocene on HOPG presents the ferrocene five-fold symmetric molecular axis oriented approximately perpendicular to the surface. The Fe L3 lineshape is similar to that of the multilayer Ferrocene Thin Film. Though the molecular orientation on Graphene/Ni(111) results similar to the HOPG case, the Fe L3 features are broader and slightly shifted. FeTPP after depositions up to 1 ML show altered Fe L3 lineshape in a Fe(II) configuration and the loss of Cl atom. For higher FeTPP thicknesses the Cl is present in the detected spectra together with a Fe(III) ion. The detected alteration of the electronic interface properties of iron porphyrin (FeTPP-Cl) on GR/Ni(111) is present also in case of HOPG substrate for coverages up to 1 ML. This coupling is mediated via the  $\pi$  electronic system of substrate, while no covalent bonds between the molecule and the substrate are established. Noticeably the ferromagnetic coupling for the molecules to the substrate occurring only when the Cl atom is detached, implies a reduction of the Fe valence state. The differences in the organic electronic properties found in the deposited layers onto the two different substrates will be discussed.

### #P138 - Pressure anisotropy and velocity shear in a plasma

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Non-gyrotropic particle distribution functions are often found in observations and numerical simulations of laboratory and space plasmas in nearly collisionless regimes. By considering the pressure tensor equation in a magnetized plasma we show how such states can be generated and maintained in the presence of a shear flow.

Novel plasma properties such as self-consistent non-gyrotropic equilibria and orientation asymmetries with respect to the magnetic field are presented.

We investigate the linear and nonlinear dynamics of the plasma waves that propagate in a non-gyrotropic plasma.

Finally we analyze, within the small Larmor radius limit, the effect of the plasma anisotropy on the linear and nonlinear development of the Kelvin-Helmholtz instability of a shear flow. This latter study is performed in the context of the interaction between the solar wind and the Earth's magnetosphere.

**#P139 - Scientific studies for the restoration of “Madonna con Bambino e San Giovanni”, a venetian school panel painting of the end of sixteenth century of Museo Diocesano of Palermo.**

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The scientific investigations aimed to the study, characterization and conservation of archaeological and artistic finds are in general based on a strong interdisciplinary approach and they allow, beside historical and artistic evaluations, to answer to questions about the dating, painting materials and technique, authors, artistic production area or movements or schools and also about authenticity of antique paintings.

The aim of this research was to assess the techniques used to create and decorate the wooden painting and to verify the state of preservation of the finishing materials of the artwork.

For that reason an integrated analytical approach based on the use of non-invasive and micro-invasive techniques was used, with the aim to obtain a characterization of the wooden panel, to elucidate the painting technique, including the stratigraphic sequence of the pigments and the organic binders employed, the state of preservation, the possible decay processes and the possible additions made during previous restorations.

The painting on wood panel (33 x 49 cm) “Madonna con Bambino e San Giovanni” represent the “Madonna della Consolazione”, referring to byzantine “Odeghetria”; it is attributed to unknown cretan-venetian artist and probably dated to the end of 16th century and it is conserved in the Museo Diocesano of Palermo.

At first the painting was analyzed by non-invasive techniques: macrophotography and photography under IR, UV and visible radiation (raking light) and Imaging techniques like IR reflectography (IRR) and false color infrared (IRFC), followed by spectroscopic ones, like reflectance spectrometry in the visible range (vis-RS) and X-ray fluorescence (ED-XRF), were chosen as informative first-step analyses. Then, after sampling, micro-fragments of the painting material were analyzed by several analytical techniques: optical microscopy, scanning electron microscopy with energy dispersive spectroscopy (SEM-EDS) and FTIR spectroscopy. Finally, for the restoration of the painting it was also used the analysis named colorimetry.

Data suggest a traditional painting technique, characterized by a single wooden panel, a thin white preparatory layer of gypsum and animal glue (< 1 mm), a dark priming (“imprimitura”), an engraved underdrawing and a paint layer composed by pigments dissolved in both egg and oil containing binding medium. The highlights (“lumeggiature”) on the dress and the nimbus are gilded with “a missione” technique (oil gilding or oil mordant or mordant gilding) while the globe in Baby Jesus hand is gilded with the technique named “a guazzo” (water gilding); in fact it is also present a reddish-brown preparatory layer (Armenian bole) composed of iron oxide with aluminosilicates.

**#P140 - Microscopic approach to investigate constitutive materials and technique of San Vito wooden pulpit of Museo Diocesano of Palermo**

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Magnificent artworks (panel paintings, architectural elements, statues, altars, sarcophagi, etc.) have been created in any culture using wood as the main constitutive material, especially for the supports. Many decorative techniques have been used on wood, with or without a preparation layer, by carving the ornamental elements, applying pigments and gold or silver leaves and inlaying ivory or mother-of-pearl, etc. Several organic binding and gluing *media* have been used: proteinaceous materials, drying oils, waxes, resins and vegetable gums.

The aim of this research was to assess the techniques used to create and decorate the wooden pulpit of San Vito and to verify the state of preservation of the finishing materials of the artwork.

The San Vito wooden pulpit (210 x 120 x 100 cm), attributed to unknown artist, coming from the oratory of San Vito and conserved in the Museo Diocesano di Palermo, has a linear structure typically nineteenth century, made by assembling many components; it is decorated by three polychrome and gilded panels representing events of the martyr life, probably dated to the end of 17th century. Micro-fragments of the support and of the painting material were analyzed by several analytical techniques: optical microscopy, scanning electron microscopy with energy dispersive spectroscopy (SEM-EDS) and FTIR spectroscopy.

Observations through the various microscopes revealed that a proteinaceous pittoric layer (probably a tempera), light green coloured, was directly applied onto the wood of the linear structure, without a preparation.

Decorative panels are well conserved and the original polychrome decorations and gilding are still preserved. In particular, the *recto* of panels is entirely covered by gold leaf, applied with the technique named "a guazzo" (water gilding) on a preparation composed by a first white layer with gypsum and animal glue and a second one with bole. The pigments are applied on gold leaf by thin and transparent brushstrokes. The palette is composed by pigments and lacquers using oil as binding medium.

Therefore the scientific analyses confirmed the preliminary observations about the pulpit, formed by a structure of the 19th century and by decorative panels of the end of 17th century, probably coming from another ancient artwork.

#### #P141 - A model for 1/f Noise in Polymer Nanofibers

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In recent years great advancements have been achieved in the field of organic electronics, driven by the strong interest in producing low-cost and flexible electronic devices [1,2]. Practical applications of these devices require understanding and controlling current fluctuations, especially in the low-frequency regime which can seriously limit the device performances. Actually, for frequency  $f < 100$  KHz, 1/f flicker noise is usually observed in all electronic devices, including nanowires, nanocrystals and organic thin films devices [1-4]. However, the changes in 1/f noise upon moving from bulk organic materials to nanostructures is still poorly investigated. This motivates the interest in studying flicker noise in nanostructures such as polymer nanofibers. Polymer nanofibers, similarly with other nanostructures with lateral confinement, generally exhibit a charge-carrier mobility significantly enhanced with respect to thin films made of the same conjugated material, as a consequence of a more ordered molecular arrangement [5,6]. Very recently we have investigated [7] the effect of lateral confinement on flicker noise in OFETs based on conductive conjugated polymers, poly(3-hexylthiophene) (P3HT) [5,6]. The noise in these devices, working in accumulation regime in air conditions, is well described by the Hooge model, suggesting a behavior dominated by mobility fluctuations. Importantly, the average Hooge parameter, controlling the relative power spectral density of current fluctuations is suppressed by about two orders of magnitude with respect to the values measured for thin-film devices based on the same active material [7]. To explain these results we have developed a resistor network model, in which the organic semiconducting nanostructures or films are depicted through a two-dimensional network of resistors. The numerical results of the model [7] agree with the experimental findings [7], supporting the role of size-confinement in organic nanostructures as effective route to improve the noise performance in polymer based electronic devices.

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#### #P142 - Non-linear transport of hot-electrons in a InP bulk operating under fluctuating fields

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The complexity of electron dynamics in low-doped n-type InP crystals operating under fluctuating electric fields is deeply explored and discussed. In this work, we employ a multi-particle Monte Carlo approach to simulate the non-linear transport of electrons inside the semiconductor bulk. All possible scattering events of hot electrons in the medium, the main details of the band structure, as well as the heating effects, are taken into account. The results presented in this study derive from numerical simulations of the electron dynamical response to the application of a sub-Thz electric field, fluctuating for the superimposition of an external source of Gaussian correlated noise. The electronic noise features are statistically investigated by computing the correlation function of the velocity fluctuations, its spectral density and the variance, i.e. the total noise power, for different values of amplitude and frequency of the driving field. Our results show the presence of a cooperative non-linear behaviour of electrons, whose dynamics is strongly affected by the field fluctuations. Moreover, the electrons self-organize among different valleys, giving rise to the reduction of the intrinsic noise. This counterintuitive effect critically depends on the relationship among the characteristic times of the external fluctuations and the temporal scales of complex phenomena involved in the electron dynamical response. In

particular, the correlation time of the electric field fluctuations appears to be crucial both for the noise reduction effect and the appearance of an anomalous diffusion effect.

#### #P143 - MHD modelling of solar coronal plasma

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In the X-ray and EUV-emitting solar corona, plasma at million degrees is confined by the solar magnetic field inside closed flux tubes, which are anchored in the photosphere. We use state-of-art multidimensional magnetohydrodynamic models to describe the interaction of erupted fragments falling back to the solar surface with the magnetic field, and other preliminary work concerning the emergence of magnetic flux tubes. We show the evolution of the plasma and predictions to be compared with X-ray and EUV observations obtained from 3D MHD numerical simulations on high-performance computing systems.

#### #P144 - Protonation Constants of Halloysite Clay Nanotubes

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Protonation Constants of Halloysite Clay Nanotubes

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Halloysite is one of the most interesting nano-structured clay materials. It is similar to kaolin but has a hollow tubular structure that can be attributable to particular crystallization conditions. Typically, halloysite nanotubes (HNTs) are formed by 15 – 20 aluminosilicate layers, has a length of  $1 \pm 0.5 \mu\text{m}$  and inner and outer diameters of 1 - 30 and 30 - 50 nm, respectively [1,2]. In each layer the SiOH and the AlOH groups are disposed on the external and the internal surfaces, respectively.

The particular structure of HNTs makes this kind of material very useful for different purposes in several fields. Among the various applications, worth of mention are: i) their use as additive for devices in the capture tumor cells in blood; ii) nanoparticles for the entrapment and controlled release of active molecules; iii) additive agents in wound and personal care; iv) sorbents for water contaminants etc [1,2]. In all these applications, the knowledge of the acid-base properties of HNTs is of fundamental importance.

The acid-base properties of HNTs have been studied by ISE- $\text{H}^+$  potentiometric titrations in NaCl medium, in the range  $0.025 \leq I / \text{mol L}^{-1} \leq 0.750$  and at  $T = 25^\circ\text{C}$ . Two functional groups indicated with  $\text{HNT}_1$  (SiOH) and  $\text{HNT}_2$  (AlOH) were considered in the analysis of the experimental data. Potentiometric data were processed with four different models previously used for the study of the acid-base properties of natural and synthetic polyelectrolytes: Högfeldt, Linear, modified Henderson-Hasselbalch and diprotic like models [3]. The results obtained with the four models for the protonation constants of  $\text{HNT}_1$  groups of HNTs were in good accordance, whilst the acid-base properties of  $\text{HNT}_2$  groups were well defined by one protonation constant calculated by processing the potentiometric titration data with the computer programs STACO and BSTAC.

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#### #P145 - Current injection from metal to MoS<sub>2</sub> probed at nanoscale

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The isolation of graphene (Gr) opened the way to the investigation of an entire class of layered materials, which are composed by the vertical stacking of 2D sheets bond by van der Waals interaction. In particular, transition metal dichalcogenides (TMD), such as  $\text{MoS}_2$ ,  $\text{MoSe}_2$ ,  $\text{WS}_2$  and  $\text{WSe}_2$ , have been recently the object of significant interest due to their semiconducting properties, which make them very attractive in electronics and optoelectronics even with respect to semimetallic Gr. As an example,  $\text{MoS}_2$  has currently being considered as a candidate for next generation post-Si CMOS technology. Due to the intrinsic stability of the material,  $\text{MoS}_2$  thin film transistors guarantee the scalability of the channel thickness down to the ultimate single layer limit. Very promising performances, such as on/off current ratios  $>10^7$  and nearly ideal subthreshold swing ( $\approx 70 \text{ mV/decade}$ ) have been already demonstrated for top gated monolayer  $\text{MoS}_2$  transistors with high-k gate dielectrics.

In spite of these great promises, processing for MoS<sub>2</sub> devices is still in its infancy and several issues, including the scalable growth of MoS<sub>2</sub> films with controlled thickness, the formation of low resistance Ohmic contacts, optimal gate dielectrics, surface passivation and doping are currently object of investigation to fully exploit the potentialities of this material.

In particular, contact resistances have been currently identified as limiting factors for MoS<sub>2</sub> transistors performances, leading to the underestimation of the field effect mobility and to a degradation of device characteristics. Experiments have shown that the Schottky barrier height between most of metals and MoS<sub>2</sub> are in the range from ~25 to ~300 meV. For high workfunction metals (Ni, Au or Pt) these values are much smaller than the ideal values expected according to the Schottky-Mott theory. Such a behavior has commonly been ascribed to a pinning of the Fermi level of metals in the upper part of MoS<sub>2</sub> bandgap. However, its origin is still matter of debate.

In this paper, we employed conductive atomic force microscopy (CAFM) to investigate the current injection mechanism from a nanoscale metal contact, i.e. a Pt coated AFM tip, to the surface of MoS<sub>2</sub> thin films exfoliated on a SiO<sub>2</sub> substrate. The analysis of local current-voltage (I-V) characteristics on a large array of tip positions on MoS<sub>2</sub> provided high spatial resolution information on the lateral homogeneity of the tip/MoS<sub>2</sub> Schottky barrier  $F_B$  and of the ideality factor  $n$ . From the histograms of the measured  $F_B$  and  $n$  values, an average Schottky barrier height of 297 meV with standard deviation of 22 meV and an average ideality factor of 1.65 with a standard deviation is 0.15 have been estimated. The implications of these lateral variations of  $F_B$  and  $n$  in MoS<sub>2</sub> nano-Schottky diodes on the electrical properties of macroscopic contacts to MoS<sub>2</sub> have been discussed also in relation with recent literature results.

#### #P146 - A bioinformatics analysis of Mass Spectrometry approach reveals a new target of A $\beta$ 42 peptide

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Proteomic changes have been described in different neurodegenerative disease including Alzheimer's disease (AD). This pathology is the most common form of dementia, and its prevalence increases exponentially with age. The patients affected gradually lose cognitive function, control over their sense of orientation, their emotions, and other aspects of behavior. Thirty-five million people are now considered to be affected by AD and this number is expected to double in the next few decades. AD cell model system in which LAN5 neuroblastoma cell were incubated for short time with a recombinant form of A $\beta$ 42 (rA $\beta$ <sub>42</sub>), a peptide involved in AD, was utilized for a study of the proteome by mass spectrometry. Furthermore, we used bioinformatics tools to mine databases and present relatedness in the form of networks, associated processes, pathways, etc. The potential modulation of pathways suggested by the similarity of GO terms and presence of protein-protein interaction networks among significantly modulated proteins was explored using the bioinformatic tool KEGG. Pathway enrichment analysis was conducted for up and down regulated protein groups, and four pathways were identified. The Spliceosome pathway identified in the under-expressed protein group was reported by KEGG to be the most significantly enriched. To confirm the effect of A $\beta$ <sub>42</sub> on the spliceosomal pathway, the level of expression of SmB/B'/N (a component of the spliceosomal machinery) was measured. Proteins were extracted from LAN5 cells treated with rA $\beta$ <sub>42</sub> at differing concentrations and times, and a Western blot was performed. SmB/B'/N levels were found to decrease in a time and dose dependent manner relative to the control suggesting that impaired splicing can occur. However, further studies are necessary to fully elucidate the the down-regulation effect of the spliceosome proteins in AD, and how this may contribute to the early event in this disorder.

#### #P147 - Dissociation mechanism of CO<sub>2</sub> under non-equilibrium discharge and post-discharge conditions

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Plasma processing of CO<sub>2</sub> in the gas phase under non-equilibrium conditions is nowadays considered as promising substitute to conventional routes to specifically tackle the rate-limiting dissociation into CO. To become an economically viable alternative to conventional fuel processing routes, the energy efficiency of the CO<sub>2</sub> processing step has to be maximised. This in turn requires a better understanding of CO<sub>2</sub> activation channels and reaction mechanisms in plasma-assisted processes. The idea to use cold i.e. non equilibrium plasmas for the CO<sub>2</sub> dissociation has a long history started with the works of Russian<sup>1-3</sup> and Italian groups<sup>4-5</sup> in the seventy, at the beginning of plasma-chemistry activities. The basic idea was the impossibility to rationalize experimental dissociation rates of CO<sub>2</sub> by using the direct electron impact dissociation process. On the contrary especially at low electron temperature ( $T_e$  of the order of 1eV) the input of electrical energy goes through the excitation of vibrational modes of CO<sub>2</sub> (in particular the asymmetric one) followed by V-V (vibration-vibration) energy exchange processes able to spread the low lying vibrational quanta over the whole vibrational ladder of CO<sub>2</sub> ending in the dissociation process. The upper limit to the dissociation rate of this mechanism, called pure vibrational mechanism can be several orders of magnitude higher than the corresponding dissociation process induced by electron impact. These simple considerations are at the basis of the numerous experimental attempts to use vibrational energy in the dissociation process rather than the direct electronic process with the conviction that the activation energy of the vibrational excitation process is much less than the corresponding electron impact process. In the present

contribution, we would like to investigate such phenomena and built up a dissociation model for CO<sub>2</sub> which takes into account CO<sub>2</sub> vibrational excited states and the strong coupling of the vibrational kinetics with the electron energy distribution function (eedf).

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### #P148 - Enhanced Efficiency of Organic Solar Cells by thiol-capped Au-Nanoparticles

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Organic solar cells (OSCs) are attracting significant interest because of their relevant features such as low cost, ease of manufacture, mechanical flexibility and lightness along with portability. Devices based on poly(3-hexylthiophene) (P3HT) as donor and soluble fullerene derivatives (PCBM) as acceptor are among the most studied, providing promising power conversion efficiency (PCE). However, low carrier mobility in heterojunction networks remain the major obstacle for improving device efficiency. Because of poor charge transport in the active layer there is competition between the separation and recombination of the photogenerated carriers. Thus, there is a need to develop strategies for increasing light harvesting by the same film thickness. Also, metallic nanoparticles (NPs) are very interesting systems due to their optical and electrical properties. In particular, metal NPs such as Au, Ag, Cu and Pt are known to show plasmon-enhanced absorption which could ensure a greater absorption and an enhanced photogeneration of mobile carriers in the heterojunction films. [1]

In this work, we present a study on the effect of thiol-capped AuNPs of various sizes in an organic solar cell. AuNPs have been obtained by laser ablation in liquid solution [2], have been functionalized both with 2-naphthalenethiol and alkanethiol having different length. In addition to bulk heterojunction structures with optimized interpenetrating network of donors and acceptor domains, we have chosen to study planar heterojunctions (PHJs), consisting of three component thin films realized by sequential deposition of P3HT, AuNPs and PCBM from orthogonal solvents.

These structures have been studied by different microscopy and spectroscopy surface tools. Results show that 2-naphthalenethiol-capped AuNPs incorporated at the P3HT/PCBM interface in planar heterojunctions ensures a more efficient charge transfer with respect to heterojunction without AuNPs. Additionally, I/V curves showed that the incorporation of AuNPs with an approximate size of 30 nm can significantly enhance the PCE from 0.7 % to 2.7. Results are discussed in terms of the dependence of fill factor, electron transfer and short circuit current on the morphological order, plasmonic and scattering properties of AuNPs in the thin films.

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### #P149 - COMPARISON OF ACTIVITY IN THE 2-PROPANOL DEHYDRATION OF SUPPORTED HETEROPOLY ACID (PHOTO) CATALYSTS AT THE GAS-SOLID INTERFACE

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2-Propanol dehydration at the gas-solid interface over supported Brønsted acid catalysts based on H<sub>3</sub>PW<sub>12</sub>O<sub>40</sub> (PW<sub>12</sub>) Keggin-type heteropoly acid was studied. A continuous flow fixed-bed reactor working at atmospheric pressure and 80 °C and isopropanol initial concentration 0.5 mM was used. Preliminary experiments were performed to find out the flow rate of the feeding gas necessary to avoid mass transport limitation phenomena and hence carry out the experiments in kinetic regime; consequently, a flow rate of 100 ml min<sup>-1</sup> was used in all the experiments. For the photo-assisted runs the reactor was also illuminated from the top with UV LEDs at different irradiances. The (photo)catalysts included bare and supported PW<sub>12</sub>. Binary materials have been prepared by impregnation and/or solvothermal treatment by using commercial supports: SiO<sub>2</sub> (Mallinckrodt), TiO<sub>2</sub> (Evonik P25) and carbon nanotubes (Sunnano) or solvothermal home prepared SiO<sub>2</sub>, TiO<sub>2</sub> or ZrO<sub>2</sub>. All the materials have been characterized by X-ray diffraction (XRD), scanning electron microscopy observations (SEM) with EDX microanalysis, specific surface area measurements and diffuse reflectance spectroscopy (DRS). The retention of Keggin anion structure throughout the synthesis of catalysts was confirmed both by FTIR and Raman spectroscopies. When the materials were also illuminated the conversion of 2-propanol and consequently the propene formation increased. Propene was the main reaction product, but also the formation of small amounts of di-isopropylether was observed; however, the various supported materials showed significant differences. The comparison of the



photocatalysts activity was performed by calculating the rate of propene formation normalized for gram of  $PW_{12}$  present in the catalyst. Indeed, the Kegginheteropolyacid species played a key role both for the catalytic and the photo-assisted catalytic reactions.

#### #P150 - Quantification of the volume and total grain size distribution of the 23 February 2013 Etna lava fountain

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The majority of the plumes produced by explosive eruptions from Mt. Etna, in Italy, are affected by winds oriented from West to East that drive the volcanic ash over the sea, allowing erupted tephra to be sampled at relatively proximal area around the volcano only, i.e. within 20-25 km from the crater. This makes the quantification of fine ash content and the Total Grain Size Distribution (TGSD) very difficult and highly uncertain. Five lava fountain episodes occurred on the New South-East Crater of Mt Etna from 17 to 23 February 2013. On the 23 February, there was a paroxysmal phase that lasted less than 1 hour, producing magma jets higher than 500 m and an eruption plume that reached at least 4-5 km above the crater. The plume was mainly advected by winds oriented from South-West to North-East. This plume produced an extended tephra fallout deposit, allowing lapilli and ash to be sampled at several locations between the slope of Etna and the Puglia region, at about 400 km from the volcano. Here we first quantify the TGSD and the fine ash content for this paroxysmal episode. Then, we use meteorological fields, column height estimation, and TGSD to initialize a computational model of tephra dispersion. Finally, the model simulations are compared with ground measurements and airborne observations allowing us to estimate Mass Eruption Rate and Total Mass through a best fit procedure.

#### #P151 - Amorphous ferromagnetism and re-entrant magnetic glassiness in $Sm_2Mo_2O_7$

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We report on the investigation of a high-quality single crystal of  $Sm_2Mo_2O_7$  by means of dc magnetometry, muon spin spectroscopy ( $\mu^+$ SR) and high-harmonics magnetic ac susceptibility [1]. The magnetic phase of the  $Mo^{4+}$  sublattice develops below  $T_c = 78$  K, in agreement with several previous reports in the literature. The  $T_c$  value would be significantly reduced by a substantial amount of  $O^{2-}$  vacancies, showing that this critical issue can be safely neglected for the currently investigated sample. Such magnetic phase for  $Mo^{4+}$  is typically discussed in the literature as a conventional itinerant ferromagnetic state. However, our results clearly detect a complicated superposition of conventional and highly disordered magnetic behaviors below 78 K sharing several common features with amorphous ferromagnetic alloys (AmFA) and with other insulating spin-glass (SGI) pyrochlore molybdates. This scenario for  $Sm_2Mo_2O_7$  is supported by the anomalously high values deduced for the critical exponents of the magnetic transition, approaching values typically reported for AmFA. These were calculated by a scaling analysis of the dc magnetization data and confirmed by  $\mu^+$ SR and first-harmonic ac susceptibility. At the same time,  $\mu^+$ SR detects a sizable static magnetic disorder at the microscopic scale resulting in strongly damped coherent oscillations in the time depolarization of the  $\mu^+$  spin. Moreover, the critical divergence of the third-harmonic component of the magnetic ac susceptibility around 80 K leads to additional evidence towards the disordered nature of this magnetic phase. Some degree of magnetic glassiness has been reported in the literature also in the metallic ferromagnetic (FMM) phase near to the metal-to-insulator boundary. However,  $Sm_2Mo_2O_7$  is located far enough from such boundary and glassy features are typically neglected in this case. Finally, as typical for several amorphous ferromagnets, a re-entrant spin-glass (RSG) phase is evidenced at low temperatures by means of both the longitudinal magnetic relaxation of  $\mu^+$  and by magnetic ac susceptibility. Accordingly, our results shed new light on the magnetic properties of  $Sm_2Mo_2O_7$  and on the overall electronic phase diagram commonly accepted for pyrochlore molybdates.

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#### #P152 - Equivalence of chemical and external pressures in RCoPnO

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We report on the local magnetic properties of the series of ferromagnetic materials  $R\text{CoPnO}$  ( $R = \text{La, Pr, Nd, Sm}$ ;  $\text{Pn} = \text{As, P}$ ) as investigated by means of muon spin spectroscopy under pressure  $P$  and ferromagnetic resonance (FMR). The effect of  $P$  is shown to be quantitatively equivalent to the chemical lattice shrinkage triggered by the different ionic radii of  $R$  ions. This is verified for both experimental dependent quantities (i. e., magnetic field at the muon site [1]) and for intrinsically material-dependent properties (i. e., ferromagnetic critical temperature  $T_c$  [2]). FMR results in a wide range of temperature, frequency and magnetic field clearly display that the chemical pressure is extremely effective in developing an easy-plane magnetic anisotropy.

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### #P153 - Microturbulence in helical and axisymmetric reversed field pinch plasmas

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In the reversed field pinch device RFX-mod (Padova, Italy), good confinement properties are achieved when the magnetic surfaces become helical. This condition causes an overall reduction of the magnetic chaos, but, at the same time, creates the physical conditions mostly favoring the onset of electrostatic/electromagnetic turbulence, e.g., the occurrence of large pressure gradients. In this contribution we review some recent findings in this field, focusing on the 3D features of the helical magnetic field, with the aim to describe its distinct properties compared to an axisymmetric plasma. We will discuss, in particular, the results on ion temperature gradient turbulence, and the effect of a finite plasma beta on electromagnetic instabilities and turbulence.

### #P154 - Astrophysical mono-protonated molecular ions: ab-initio simulation of x-ray photoabsorption spectra

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The detection through spectroscopic signatures of molecular ions in interstellar media is of prime importance due to their potential role as precursors of larger molecules<sup>1, 2</sup>. We focused here on the K-shell photoabsorption spectroscopy of the hydride monoprotinated molecular ions  $\text{CH}^+$  and  $\text{OH}^+$  and the L-shell of  $\text{SiH}^+$  (100- 550 eV, soft X-ray range)

Experimental data for the monoprotinated molecular ions  $\text{SiH}^+$ ,  $\text{CH}^+$  and  $\text{OH}^+$  were recorded on the PLEIADES beamline at the SOLEIL synchrotron facility using a merged beam technique with an electron cyclotron resonance ion source (ECRIS).

In our study, we have simulated the photoabsorption spectra of the species presented above using a combination of post Hartree-Fock and nuclear wavepacket methods. More precisely, the calculations of the potential energy and dipole transition curves were performed using the Configuration Interaction method and Spin-orbit coupling taken into account through the Breit-Pauli operator. The relaxation energy which is expected to be large for core-excited states is accounted by the use of molecular orbitals optimized for the first core-excited state. Core hole lifetime and nuclear dynamics are explicitly included in the calculations of the photoabsorption spectra.

In order to take into account of the plasma temperature on the photoabsorption profile (distribution of electronic states), we have evaluated the energies of the low-lying different spin states (singlet and triplet) at the DFT (Density Functional Theory) level of theory using the B3LYP exchange-correlation functional.

Our results compare quantitatively with the experiments. They allow the attribution of the experimental spectroscopic lines and the population of the lowest singlet and triplet states. The satisfactory results obtained encourage us to extend further the study to the multiprotinated molecular ions  $\text{SiH}_n^+$ ,  $\text{CH}_n^+$ ,  $\text{OH}_n^+$  ( $n=2,3$ ).

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**#P155 - Silicon nanowires integrated in solar cells.**

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Nanostructured materials attract enormous interest for application in PV for their numerous intriguing properties. Quasi-zero dimensional (0D) nanostructures such as Si nanocrystals (Si-NCs), thanks to the band-gap widening effect, effectively convert in electric energy photons in the blue part of the solar spectrum, thus decreasing the efficiency losses related to carriers thermalization and for this reason can be exploited in multi-junction solar cells, although the Si/SiO<sub>2</sub> interface present at the Si-NCs surface provides an effective energy barrier for the carrier transport [J. Appl. Phys. 108 (2010) 023701]. Also quasi-one dimensional (1D) Si nanostructures such as nanowires have demonstrated their potential in PV because their architectures allow, with respect to the planar Si, increased light absorption due to their exceptional light harvesting properties. For the NWs to become applicable to PV, cost-effective synthesis methods, providing at the same time control on their morphological characteristics, must be pursued. Currently most of the synthesis methods require high temperature deposition systems or provide poor control on their surface roughness. In the fabrication processing of nanostructure-based devices the doping step is crucial as well. The requirements are: absence of crystal damage, control of doping profile at nm level, possibility to obtain high dopant concentrations and conformality. In this work a method to grow NWs by using a low temperature CVD system is used. Moreover, an innovative method to dope the nanostructures is proposed, based on the formation of a self-assembled monolayer (SAM) of dopant precursor molecules via silylation from liquid solutions [Nat. Mat., 7(2008) 62, Phys. Stat. Sol. A (2015), in press]. Arrays of SiNWs with  $1 \times 10^{10}$  cm<sup>-2</sup> density, 1 μm length, up to 60 nm diameter have been obtained, ex-situ doped by silylation and finally integrated as top active layers inside the cells [Sol. En. Mat. Sol. Cells 132 (2015) 118]. The results show that the NWs present highly controlled atomically flat surface after the deposition and after the doping step, and the NWs devices show higher short circuit current than the reference cells.

**#P156 - The self-assembling anisotropic particles: nematic phase**

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Self-assembly-driven nematisation occurs when basic building blocks, due to anisotropic particle-particle interactions, form linear semi-flexible aggregates, which may mutually align to form nematic liquid crystals (LCs). Since scattering experiments easily provide the information on system structure in the form of structure factors, it is necessary to develop a formalism to theoretical calculations of density-density correlations based on the results of the predicted self-assembly and phase behaviour. We investigate the nematic LC formed by sphere-cylinders that self-assemble in linear chain structures and trying to answer the question: How are the spatial correlations in the system influenced by the nematic order parameter? To do so, we distinguish between the spatial correlations in the plane perpendicular to the crystalline axis, and in the direction parallel to the latter.

Following this separation, we put forward a theoretical approach to calculate radial distribution functions (RDFs) and structure factors (SFs) separately. We show that the RDFs in the parallel case can be described using a superposition of a chain model [1] and Onsager distribution [2], whereas the RDFs in the perpendicular case turn out to be that of the soft disks [3]. After that SFs are calculated using different methods of the statistical physics. We test our theoretical methods against the results of canonical NVT Monte Carlo simulations of hard cylinders with attractive sites on their bases [4] and perform detailed analysis.

We conclude that even if the nematic ordering in the system is high, the imperfection of the liquid crystalline phase is strongly reflected and even magnified in the pair distributions. Our theoretical approach is rather general and as an input parameter uses only the particles' shape, volume fraction and the bonding free energy, which is why it is applicable to any system where the equilibrium self-assembly in chains causes the isotropic-nematic transition.

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**#P157 - Self-assembling in the system of nanocylinders and nanodisks**

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The process of self-assembly is a key to design and control various systems, and as such it has recently become a subject of interest in physics, chemistry and biology.

In the present theoretical study we focus on the two type of building blocks: cylinders and discs (magnetic and nonmagnetic), that can form different types of clusters. First of all we investigate possible structural change in the system with changing particles' parameters, such as: size, shape and value of the magnetic moment (for magnetic particles). After that we present the theoretical models for calculation different macroproperties (for example initial susceptibility for magnetic particles) and analyse them as functions of aforementioned particles' parameters and concentration. Our theoretical results are supported by an extensive comparison of the theoretical predictions to the results of computer simulations.

We conclude that self-assembly can change macroscopic behaviour nanocylinders and nanodisks systems. This may be very important for the syntheses of new materials with controllable microstructure and macroproperties.

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### #P158 - Alpha-Lactalbumin amyloid fibril formation and interaction with Giant liposomes

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Several neurodegenerative diseases like Parkinson's and Alzheimer's disease or type-II diabetes are associated with the formation and deposition, in human organs and tissues, of large amounts of insoluble and highly ordered protein aggregates, known as amyloid fibrils. Hence, specific interest in recent biomedical research has been focused on protein aggregation. In the last years, several works have assessed that the interaction of amyloidogenic proteins or aggregates with cell membranes is critical in the onset and progression of disease.

We here present an experimental study on a model protein, alpha-lactalbumin ( $\alpha$ -La).  $\alpha$ -La is a small acidic  $\text{Ca}^{2+}$ -binding whey protein, widely studied for its potential pharmaceutical and medical applications and used as a model for molten-globule analysis. Using spectroscopy and microscopy techniques, we analyze the fibrillation mechanisms and the interaction of this protein, in different aggregation states, with model membranes. Thermally induced  $\alpha$ -La amyloid formation was analyzed by means of light scattering and in situ Thioflavin T (ThT) fluorescence measurements, in different conditions. To probe the secondary structure and morphology of the supramolecular structures, the aggregates were characterized by FTIR absorption spectroscopy and by confocal fluorescence microscopy. This multi-technique approach is used to analyze the protein amyloid formation and to characterize the different aggregation states during supramolecular assembly kinetics. The interaction of  $\alpha$ -La aggregate species and giant liposomes as model membranes was investigated by means of Laurdan dye and two-photon microscopy. This approach allows quantifying the changes in membrane fluidity upon protein aggregates addition simultaneously with the visualization of morphological changes in model vesicles.

### #P159 - Toward metrological-grade sub-Doppler THz spectroscopy

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High precision THz molecular spectroscopy promises amazing scientific and technological applications, provided that sources with suitable high power, wide tunability and narrow linewidth, such THz Quantum Cascade Lasers [1] are available. In this context, the first application of a QCL phase-locked to a free-standing THz Frequency Comb Synthesizer (FCS) [2] was recently demonstrated, achieving a state-of-the-art accuracy of  $4 \times 10^{-9}$  in the determination of the absolute frequency of a THz transition [3]. In this experimental report the overall accuracy was limited by the resolution of the Doppler-broadened direct-absorption spectroscopy adopted therein. As a consequence, the the development of high-resolution THz spectroscopic techniques, such as saturated-absorption spectroscopy (SAS), is a mandatory condition for further accuracy improvements.

We therefore report on the evidence of saturation effects in a rotational transition of  $\text{CH}_3\text{OH}$  around 2.55 THz, induced by a free-running continuous-wave QCL [4], confirming the feasibility of QCL-based subDoppler spectroscopy, once provided that the QCL emission linewidth is comparable with, or narrower than the Lamb-dip width. The QCL emission is used for direct-absorption spectroscopy experiments, allowing to study the dependence of the absorption coefficient on gas pressure and laser intensity. A saturation intensity of  $25 \mu\text{W}/\text{mm}^2$ , for a gas pressure of 17  $\mu\text{bar}$ , is measured.

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### #P160 - Low environmental impact materials for cleaning of artistic surfaces

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The operation of cleaning has always been a difficult task to perform on artworks. The need to use both controlled and selective cleaning methods, in order to minimize the impact of the treatment over the artistic surface, has guided many of the researches in conservation field. A great part of the works that tackled this problem concentrated on finding new application methods that use traditional solvents trapped in retentive systems that reduce their diffusion rate into the inner pictorial layer (also called "solvent gels"<sup>[1]</sup>). Despite being effective in performing with efficiency the cleaning task, these systems carry with themselves all the health safety issues related to the use of those potentially hazardous traditional organic solvents.

Taking this into account, an attempt to use solvents having lower environmental impact and increased health safety for the end user, should be carried out in order to preserve both the restorer and the artwork. Three of these "green" solvents are 1,3-dioxolane, methylal and propylene carbonate. In spite of their use in cosmetics and personal care formulations<sup>[2]</sup>, at the moment they aren't commonly employed by restorers during cleaning campaigns.

In this work, the performance of 1,3-dioxolane/methylal and propylene carbonate, is evaluated over a wooden painted tablet that had been covered with a thin layer of a protective varnish during a previous conservation intervention performed in the Sixties. Removal of this varnish has been considered on behalf of its yellowing degradation process, that caused chromatic changes over all the pictorial layer. The cleaning process has been followed by FT-IR external reflectance spectroscopy, directly in situ, using a portable spectrometer. In this study, it is also considered the use of a new supportive material that can permit to obtain a higher control of the cleaning process, respect to the use of the "free" solvents. Furthermore, attention has been given to the development of the application method for these systems; comparison with traditional solvents and application methods has also been done, both in terms of cleaning efficiency and lingering of residues of the cleaning material.

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### #P161 - Distinguishing stochastic noise from other kinds of dynamics in a time series

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The divergent rate method [1] can be used to determine the maximum Lyapunov exponent of a system out of a time series generated by that system, provided a suitable embedding is applied: the Lyapunov exponent corresponds to the slope of the growing section of the diagram  $L(k)$ , namely the average of the logarithm of the ratio between the distance of two points after  $k$  steps and their initial distance. This last quantity is constrained to be within a given "shell".

We show how the value corresponding to the asymptotic behaviour of a diagram, namely  $L(k)$  at large  $k$ , allows to distinguish stochastic noise from other kinds of dynamics in a time series. We analytically compute the asymptotic value in case of a random series as a function of the embedding dimension  $m$ .

Our result can provide a new tool in the quest for a reliable method to distinguish noise from chaos in a time series.

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### #P162 - Resveratrol loaded in liposomes induces chain packing modification

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Resveratrol is a phytoalexin naturally present in some plants such as grapes, peanuts, mulberries and red fruits. It is also found in beverages, particularly red wine. The molecule has beneficial health effects, including antioxidant, antiatherosclerotic, cardioprotective, and chemopreventive properties. Cellular targets for these health benefits are nucleic acids, membrane proteins and lipid bilayers. In spite of the positive effects, resveratrol shows low solubility in aqueous media, and consequently in biological fluids. In addition, the conversion of the *trans* form into the biologically inactive *cis* isomer reduces resveratrol activity. Both limitations are overcome by loading the polyphenol into water-soluble, biocompatible carriers such as proteins and lipid bilayers.

We present the results of a spin-label ESR and DSC study on the interaction of resveratrol with membrane models composed by DPPC lipid, one of the most abundant in cell membranes.

At temperature through the gel phase of DPPC bilayers, the addition of resveratrol markedly restricts the motion of chain-end labelled lipids, abolishes the profile of increasing mobility and reduces the order along the acyl chains, whereas it does not affect the rotational mobility and the fluidity gradient in the fluid phase.

DSC endotherms indicate that resveratrol at low concentration influences the pre-transition, which is abolished from 5 mol% onwards, whereas it has negligible effects on the main transition. At high concentration (up to 50 mol%), resveratrol reduces the main transition temperatures and the cooperativity of the transition.

The results indicate that the molecule can be loaded up to high concentration in the lamellar assemblies of DPPC liposomes and induces a gel phase with interdigitated acyl chains.

#### #P163 - Singular field energy densities at boundaries or near point-like field sources

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We discuss the problem of the divergences of field fluctuations near a point-like field source or at boundaries in the vacuum. We first consider the case of a metallic boundary, and discuss the singular behaviour of the electric and magnetic energy densities at the interface between the metallic boundary and the vacuum space. Then, we investigate the field fluctuations near a point-like field source, such as an atom, and show that also in this case the field energy densities exhibit divergences at the source position. We show, in both cases, that these singularities are at the origin of the known discrepancy between the value of the total electromagnetic field energy, calculated as the ground-state expectation value of the field Hamiltonian or as the space integral of the electromagnetic energy density.

We show that this singular behaviour disappears when extended field sources or fluctuating boundaries are considered. Specifically, we discuss the case of a reflecting boundary oscillating around its equilibrium position and show that the motion of the wall modifies the energy density of the field and smears out its singular behaviour.

#### #P164 - Novel approach for a user-friendly aptamer-based detection kit for *Staphylococcus aureus* in biological fluids

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*Staphylococcus aureus* is a common Gram-positive pathogen, present in inadequately treated food, causing a wide spectrum of diseases and one of the leading causes of mortality and morbidity in health care associated infections. Nowadays, antibiotic-resistant strains of *S. aureus* are seriously challenging global monitoring platforms. Currently, the most important detection methods are classical cultures and biochemical tests. However, they are time-consuming and not highly sensitive. For this reason, there is currently a huge demand for rapid methods for *S. aureus* detection to be incorporated into point-of-care diagnostic systems.

A novel and highly performing approach is offered by aptamers, tailored DNA or RNA sequences acting as artificial recognition elements for conserved epitopes on the bacterial surface. The technological challenges for the use of aptamers-based biosensors in the clinical practice is the lack of materials for their high-density immobilization.

Since aptamers interacting with *S. aureus* are already known, we took advantage of this knowledge tackling two principal drawbacks of the aptamer-based biosensor available to date: the lack of materials for high-density surface immobilization with aptamers and the restriction in the user-friendly read-out of the detected molecules.

We developed a device where the detection of *S. aureus* is based on the displacement by bacteria of a fluorescein-labeled peptide that selectively recognizes the aptamer. Nanostructured zirconium dioxide supports have been used for immobilizing the aptamers, allowing high-density immobilization while retaining their functionality. The displacement of the peptide is associated with a detectable change in the fluorescence of the labeled peptide. For the design of peptides specific for *S. aureus* aptamers we exploited the energy-based amino acid-base recognition code, previously obtained for several protein-DNA complexes.

This approach can be expanded towards any biological agent for which selective aptamers have been identified, allowing immediate applications in clinical and environmental monitoring, particularly in those conditions where a rapid and specific detection of one or multiple bacterial agents is needed.

**#P165 - Spin transfer torque with excitons***Massimo Rontani - CNR-NANO Research Center S3**Other Authors: K. L. Vendelbjerg (CNR-NANO S3), L. J. Sham (Dept of Physics, University of California San Diego)*

The phenomenon of spin transfer torque (STT) between a small ferromagnetic (FM) domain and a spin-polarized current plays a crucial role in spintronics. In this work we investigate theoretically the effect of STT induced by a flow of spin-polarized quasiparticles through a thin ferromagnetic layer when the ground state is a Bose-Einstein condensate of excitons produced by a coherent optical field.

We consider a one dimensional scattering model with mirror symmetry which consists of a thin ferromagnetic layer sandwiched between two semiconductors (SC). The semiconductors are treated within a two-band model in the effective mass approximation. The thin ferromagnetic layer acts as a spin-dependent scattering center for the quasiparticles, which are the elementary excitations of the excitonic ground state. Excitons are indeed continuously created through irradiation by an external laser in a steady state regime. By considering elastic scattering at equilibrium and matching the wave functions across the SC-FM junction, we work out the scattering matrix and compute the STT for both one and three dimensional structures. We find a sharp dependence of the STT on the quasiparticle energy close to the edge of the transport gap. Here we observe a quenching of STT which is a peculiar coherence effect of the exciton condensate. This behavior could be useful for spintronics applications.

**#P166 - Tunneling spectroscopy of few interacting Fermi atoms***Massimo Rontani - CNR-NANO Research Center S3**Other Authors: Pino D'Amico (CNR-NANO S3)*

We develop a theory for the tunneling of a single atom or a correlated pair out of a trap containing few interacting cold atoms. In the repulsive regime the quasiparticle wave function, dressed by the interaction with the companion atoms in the trap, replaces the non-interacting orbital at resonance in the tunneling matrix element [1]. The computed tunneling time for two  $^6\text{Li}$  atoms agree with recent experimental results [2], unveiling the 'fermionization' of the wave function and a novel two-body effect [1]. For attractive interactions we add the possibility that two atoms tunnel as a bound pair [3], leading to qualitative agreement with the measured two-atom decay time [4]. Using exact diagonalization [5] to treat up to six fermions with balanced spin population, we find evidence of BCS-like pairing [6]. For moderate interaction strength, we reproduce the even-odd oscillation of the separation energy observed in [4]. For strong interatomic attraction the arrangement of dimers in the trap differs from the homogeneous case as a consequence of Pauli blockade in real space.

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**#P167 - Modeling monoclonal antibodies with patchy particles***Michela Ronti - University of Vienna**Other Authors: Emanuela Zaccarelli ('Sapienza' University of Rome, CNR-ISC Rome), Nicholas Skar-Gislinge (Lund University, Novo Nordisk Denmark), Peter Schurtenberger (Lund University), Anna Stradner (Lund University)*

Modeling monoclonal antibodies with patchy particles

Combining direct analytical theoretical calculations and canonical Monte Carlo simulations we have studied the solution behavior of a monoclonal antibody over a large concentration range, in order to investigate the consequence and nature of the protein-protein interactions.

We have used a simple colloidal patchy model, in order to obtain analytically the thermodynamic properties (through the Wertheim theory [1]) and to obtain the connectivity properties (using the Hyperbranched Polymers Theory [2]). We have also used Monte Carlo simulations to verify the results predicted theoretically.

We are currently working to better understand the protein-protein interactions and to study analytically the structure factor. Our final aim is a mapping of the numerical and theoretical results with the experimental results of the group of Lund University.

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**#P168 - Molecular Dynamics simulations of hydrogen and oxygen atom on silica surface***Maria Rutigliano - CNR-NANOTEC*

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The interaction of plasmas with surfaces can lead to different surface processes active in different collisional energy regimes according to the behaviour of the gas-phase species and substrate involved. In particular, atom recombination at surfaces can be an effective source of roto-vibrationally excited molecules and, at the same time, an effective process for surface atom abstraction and atom removal from the plasma region [1]. Such processes have a strong impact on the physical-chemistry of the bulk region and at the plasma-surface interface. In fact, it is well established that the reactivity of molecular plasmas under low-pressure, low-temperature conditions depends on, and is often controlled by, the formation of energetically vibrationally activated molecules [2]. Therefore, it is important to understand the processes by which one can store vibrational quanta in the vibrational manifold of the active molecules in the plasma or gaseous media.

This contribution is focused on the molecular surface processes due to the interaction of a flux of H and O atoms colliding with a silica surface at low-collisional energies (0.1-3 eV). Hydrogen and oxygen plasmas are currently of great interest in different research areas of fundamental and technological interest such as microelectronics, nano-medicine, modern solar cells, fusion reactors, astrophysics and aerothermodynamics.

We will present the results obtained during the last years by our group in the study of the interaction of atoms of H and O on a silica surface based on analytical DFT Potential Energy Surfaces [3, 4]. Molecular Dynamics calculations have been performed using a semiclassical collisional method that provides a detailed knowledge of the multiphonon inelastic processes that assist the dynamics of the chemical and physical phenomena due to the chemi-/physic-sorption of atoms and molecules on substrate [5].

In particular, results concerning the recombination of H [4] and O [6] atoms on the silica surface will be discussed, in a comparative manner, respect to the recombination probabilities and coefficients, energy distribution in the final states and vibrational distributions of the formed molecules.

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### #P169 - Localized Surface Polaritons in J-Aggregate Nanostructures

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We show, by accurate scattering calculations, that nanostructures obtained from thin films of J-aggregate dyes, despite their insulating behavior, are able to concentrate the electromagnetic field at optical frequencies like metallic nanoparticles. Specially we investigate ultrathin nanodisks and nanodisk dimers which can be obtained by standard nanolithography and nanopatterning. J-aggregate nanoantennas could be exploited for the realization of switchable localized surface resonances for nanophotonic devices and could represent a low-cost solution for improving photovoltaic devices and for the realization of efficient artificial photosynthetic light-harvesting antennas. These results, in view also of the huge variety of organic dyes that can aggregate and their chemical exibility, hold the promise to greatly enlarge the availability of new plasmonic materials with diereent properties with respect to noble metals. For example J-aggregates display attractive nonlinear optical properties which could be exploited for the realization of switchable localized surface plasmons [1].

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### #P170 - Estimation of the optical parameters of atmospheric aerosol from Lidar signals by iterative inversion methods

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Atmospheric aerosol are particles systems of different type (anthropogenic and natural), whose presence causes changes in the physical properties of the atmosphere, with important implications on climate and the human health. Therefore the request of a greater care in the their knowledge and characterization therefore is increasing.



At present the Lidar technology is the best way to study the atmosphere and its composition. Lidar systems are used in the monitoring of air quality and to control the emissions of industrial plants, airport and city areas.

The Lidar technology examines the backscattering profiles obtained by the interaction between laser light and the atmospheric components, as a function of the altitude and time. In order to obtain information about the aerosols from these profiles, the optical parameters  $\alpha$  (extinction coefficient) and  $\beta$  (backscattering coefficient) must be extracted from lidar data.

However the inversion of the equation describing the lidar signal is a ill-posed mathematical problem and its solutions have a non linear dependence on the measurements uncertainties.

A new iterative method for the inversion of Lidar equation has been implemented. Its applications to synthetic as well to real cases is presented together with an analysis of the accuracy of the proposed method.

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#### **#P171 - Hybrid nanoassemblies of core-shell silica nanoparticles and hyaluronic acid: a study of energy transfer processes and cellular uptake**

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Nowadays the use of surface engineered nanoparticles for the controlled delivery of biomolecules to cells draws more and more interest, due to the challenging need of enhanced drug bioavailability, efficiency of release and triggered cytotoxicity.

In the present study we addressed the cellular uptake of hyaluronic acid (HyA) and its fluorescent derivatives (HyAF) by means of core-shell silica nanocarriers (NP). HyA is a disaccharide glucuronic acid/N-acetylglucosamine polymer, which offers high potentiality of conjugation with drugs, prodrugs, proteins or lipids via the carboxylate group on the glucuronic acid residue, the primary hydroxyl on the N-acetylglucosamine moiety, or via reductive amination chemistry through the reducing end of HyA. The tailoring of HyA hydrogel physico-chemical properties (chemistry, surface charge, hydrophilicity, viscoelastic character) as well as those of the silica nanocarriers (including the nanoparticle surface decoration with PEG, carboxy and amino-groups, and the functionalization in the core with dye molecules) was scrutinized to drive the controlled uptake of HyA and HyAF compounds in HeLa and neuroblastoma cells.

The physicochemical characterization of the hybrid bio-organic/inorganic multifunctional nanoassemblies of HyA/NPs and HyAF/NPs was carried out by dynamic light scattering and zeta potential measurements, for the hydrodynamic size and surface charge determination, atomic force microscopy, for topography and nanomechanical analyses, UV-visible and fluorescence spectroscopy, for the investigation of electron- and energy-transfer processes. The cellular response to the treatment by the differently functionalized hyaluronic acid/silica nanoparticle systems was scrutinized by viability assays and live cell imaging confocal microscopy. Results demonstrated the high potentiality of the used strategy to finely control the biomolecule-cell interaction.

#### **#P172 - Lipid-wrapped polymeric cyclodextrin nanoparticles for encapsulation of curcumin and smart delivery to cells**

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Cyclodextrins are a family of cyclic oligosaccharides with a hydrophobic central cavity and a hydrophilic outer surface. In the pharmaceutical industry cyclodextrins have mainly been used as complexing agents to increase aqueous solubility of poorly soluble drugs, thus to increase their bioavailability and stability. Curcumin is a polyphenol molecule, with a variety of pharmacologic properties, including antioxidant and anti-inflammatory activities.

In the present work polymeric nanoparticles of  $\beta$ -cyclodextrins (CDp) were used as nanocarriers for curcumin for hosting in supramolecular complexes the drug, which is poorly insoluble in aqueous solution. Moreover, since cyclodextrin molecules are relatively large with a number of hydrogen donors and acceptors and, thus, in general they do not permeate lipophilic membranes, the curcumin-CDp complexes were encapsulated in lipid vesicles, to improve the cell permeability. The loading and release of curcumin in both CDp-curcumin complexes ( $[\beta\text{CDp:curc}]$ ) and the complexes encapsulated into the lipid membranes ( $\text{SUV}[\beta\text{CDp:curc}]$ ) were characterized by a multi-technique approach based on spectroscopic methods (UV-visible, fluorescence, NMR), dynamic light scattering and zeta potential respectively for hydrodynamic size and surface charge, and atomic force microscopy in liquid.

Cellular experiments with the human RPE cell line (ARPE-19) were performed by confocal microscopy and cell viability assays. Results point to the promising potentialities of the developed nanoplatform for the controlled delivery of curcumin in application of inflammatory ocular diseases.

**#P173 - Plasma functionalization of gold nanoparticles for biosensing applications**

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The present investigation deals with the functionalization of gold nanoparticles (Au NPs) with primary amine-based plasma polymer films (NH<sub>2</sub>-PPF), to improve their properties for bioanalytical applications.

Cyclopropylamine (CPA) plasma polymerization, in pulsed and continuous wave radio frequency discharges, was employed to growth CPA amino-based PPFs coatings (18 nm) onto Au NPs of 12 nm of diameter deposited on glass and silicon substrates. A multi-technique investigation, based on FT-IR and XPS spectroscopies, AFM and SEM microscopies and ToF-SIMS spectrometry, revealed peculiar features of the CPA PPFs.

In particular, by FT-IR it was possible to obtain an overview about the rich chemistry of such PPFs, and by XPS, combined with chemical derivatization by using the reagent TFBA, it was possible to quantify unambiguously the surface -NH<sub>2</sub> amount. For testing the response in a biological environment, the behavior of the PPFs in phosphate buffer saline solution was studied upon 24 hours of immersion. The decrease of thickness occurred, related to a restructuring of the PPF structure induced by the diffusion of the solvent in the polymeric network. Such an effect of diffusion strongly depends on the cross-linking density of the PPF, characterized in the present study by ToF-SIMS. Despite such structural rearrangements, SEM does not show any evidence of delamination or damage caused after 24 hours of ageing in PBS. Results are therefore very promising for biosensor applications, as demonstrated by proof-of-work experiments with proteins and peptides.

**#P174 - Palladium clusters on BNNT as catalysts for biomass conversion**

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The construction of a heterogeneous catalytic systems by a bottom-up approach is a fascinating strategy well assisted by molecular level characterizations. In this sense, DFT investigations can be used with predictive and descriptive purposes both for the treatment of the catalyst/support and for the substrate/catalyst characterization. This should be particularly useful for highly perspective but scarcely treated systems such as boron nitride based supports. Among these, boron nitride nanotubes (BNNT) have been demonstrated to have high chemical and thermal stability as well as great mechanical strength and high thermal conductivity.[1] Moreover, a high affinity toward hydrogen [2] as well as a moderate one to carbon dioxide, suggest their possible use as support for biomass conversion catalysts.

In this work we studied through computational methods, how small Pd<sub>2</sub> up to Pd<sub>9</sub> clusters can nucleate and grow on a BNNT support; the study of the interaction occurring between palladium clusters and the support can be highly revealing for the possible production of shape and size-controlled nanoparticles. We demonstrated that the migration process of a single palladium atom on the BNNT is not highly energy demanding and can be represented as a hopping mechanism between boron and nitrogen. A model was found for the interpretation of the growth energetics, showing that the process is generally favoured increasing the cluster size. Results from the adsorption of oxygenates compounds, as model for biomass feedstocks,[3] are discussed.

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**#P175 - Theoretical Investigation of Aqueous Phase Reforming of 1,2 Propanediol over a Pt catalyst**

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Aqueous Phase Reforming (APR) process is one of the most efficient solution for producing hydrogen from biomass renewable feedstocks, such as polyalcohols. [1] Generally the reaction is catalyzed by supported platinoid metals and among these platinum has been recognized as the most active and selective toward the production of hydrogen. However, due to its really high complexity, the reaction mechanism is today poorly understood.

DFT methods can be useful for understanding the APR catalytic mechanism at atomistic level. A detailed mechanistic study was carried out using a Pt<sub>30</sub> cluster for the modelization of the catalyst and 1,2 propanediol (1,2PDO) as a model feedstock for the APR. Even for this simple molecule five chemically different hydrogen atoms can be recognized which lead to five different reaction

paths. The activation energy required for the methylic C-H bond cleavage is approximately 40 kJ mol<sup>-1</sup> higher than the HOCH-H and HOC-H bond breakings. This effect arises directly from the presence of the OH group that reasonably enhances the possibility of the C-H bond to break. The key step of the reaction seems to be the formation of the unsaturated 1,2 propenediole species that, if coordinated to the catalyst surface, can be reformed through a C-C bond cleavage or can be easily converted to ketonic species, which are experimentally found as byproducts. [2] The C-C bond cleavage is the rate determining step requiring 95.7 kJ mol<sup>-1</sup>.

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#### #P176 - Gravitational Instabilities associated with volcanic clouds: new insights from experimental investigations

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Gravitational instabilities are often observed at the bottom of volcanic plumes and clouds generating fingers that propagate downward enhancing sedimentation of fine ash. Regardless of their potential influence on tephra dispersal and deposition, their dynamics is not completely understood, undermining the accuracy of volcanic ash transport and dispersal models. Here we present new laboratory experiments that investigate the effects of particle size, composition and concentration on finger dynamics and generation. The experimental set-up made at the laboratory of the University of Geneva consists of a Plexiglas tank of 50 cm x 30.3 cm x 7.5 cm equipped with a removable barrier for the partition of two separate layers. The lower partition consists of a solution of water and sugar and is therefore characterized by a lower density than the upper partition which is filled with water and particles. The upper layer is quiescent (unmixed experiments), or continually mixed using a rotary stirrer (mixed experiments). After removing the horizontal barrier that separates the two fluids, particles are illuminated with a 2W Nd-YAG laser named RayPower 2000 and filmed with a HD camera (1920x1080 pixels). Images are analysed by the Dynamic Studio Software that is a tool for the acquisition and analysis of velocity and related properties of particles inside the fluids. Each particle that follows the flow and scatters light captured by the camera is analysed based on velocity vectors. Experiments were carried out in order to evaluate the main features of fingers (number, width and speed) as a function of particle type, size and concentration. Particles include glass beads with diameters < 32 µm, 45-63 µm, and 63-90 µm and andesitic, rhyolitic, and basaltic volcanic ash with diameters < 32 µm, 45-63 µm, 63-90 µm, 90-125 µm, 125-180 µm and > 180 µm. Three concentrations in the upper layer were considered to generate fingers: 3 g/l, 4 g/l and 5 g/l.

#### #P177 - Lidar measurements during the 16 December 2013 explosive activity at Mt. Etna, in Italy

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A new lidar named AMPLE has been installed at Mt. Etna, in Italy. The lidar is a portable multiwavelength scanning system able to carry out high quality 3D map of particle optical and microphysical properties and detect their time evolution. The laser source is a doubled and tripled diode pumped Nd:YAG laser, with a repetition rate of 1KHz. The lidar system detects the elastic returns at 355 nm and the N2 Raman lidar echoes at 386 nm. Each signal is acquired with a raw spatial resolution varying from 30 cm to 30 m. The lidar system is operated at Serra La Nave, 7 km away far from the Etna summits, and, during the winter seasons, at the INAF-Astrophysical Observatory in Catania. Lidar measurements caught explosive activities from the New South East Crater of 16 December 2013 between 11:50 and 17:30 UTC. The analysis of lidar profiles measured in the late part of the afternoon allowed to detect an aerosol layer located at high altitude that was related to the emission of fresh volcanic ash from a new eruptive vent located at the north east side of the New South East Crater. Elastic/Raman lidar measurements allowed to measure simultaneously the aerosol backscattering and the extinction coefficients at 355 nm and profiles of lidar ratio. Calibrated particle linear depolarization values in the plume were obtained from lidar profiles measured in the parallel and perpendicular polarized channels at 355 nm and allowed to distinguish fresh volcanic ash in the detected plume.

#### #P178 - Specific and aspecific effects in bioprotection of Myoglobin: a comparison between glassy trehalose and gelatin crowding.

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Preservation of biological molecules is a relevant topic both for its technological applications and for the challenges in understanding the mechanisms at its basis, either in vitro or in vivo. Saccharides, and in particular trehalose, have been widely

studied for their effectiveness in biopreservation, and various hypotheses have been prompted to explain the underlying molecular mechanisms, based either on specific, water-mediated, interaction with the embedded biomolecules or on the aspecific alteration of the physical properties of the matrix. High molecular-weight polymers are also utilised as biomaterial stabilisers in pharmaceutical or food technology, mainly because of their concurrent positive effects in system rheology. However, their preservation efficiency is not likely to depend on specific interactions with the embedded biomolecules, but only on crowding effects, as studies on polysaccharides and disaccharides/polysaccharides mixtures.

Here we present a study on myoglobin (Mb) preservation in gelatin (hydrolysed collagen), in crowded Mb-only system, and gelatin/trehalose matrices. Gelatin was chosen for its simple structure, which is analogous to a simple polymer, and its great resistance to denaturation. Myoglobin was chosen as a well characterised probe molecule, both in the oxidized met-Mb form and in the reduced carboxy form (MbCO). Data from Differential scanning calorimetry (DSC) and UV-Visible Spectroscopy are reported and compared with results already reported for Mb/trehalose systems [1].

DSC measurements were performed at various water content and allowed to obtain the denaturation temperature of Mb, pointing out a difference between trehalose matrices, who always stabilise Mb, and gelatin-containing systems, in which a destabilisation at high-to-middle hydration is in contrast with a stabilisation at very low water content. Spectroscopy measurements were performed on systems dried up to 66 days at 80°C under vacuum to test the effects of sustained stress. Through the spectroscopic study of CO loss from MbCO it was also possible to differentiate massive denaturation from functional denaturation. Overall, results show that trehalose biopreservation is more effective in the long-range and against functional denaturation, while crowding-induced preservation provides a better performance against abrupt massive denaturation and/or aggregation.

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#### #P179 - Coupling GC/MS and gas sensors for monitoring chronic health conditions in Ambient Assisted Living solutions

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The constant increase of the life expectancy and the consequent aging phenomenon will inevitably produce in the next 20 years deep social changes that lead to the need of innovative products and services for elderly people, focused to maintain independence, autonomy and, in general, improve the health conditions and wellbeing. The goal is to allow individuals to have an active role in self-managing their own health, limiting the doctor intervention, and in maintaining good health conditions.

Ambient Assisted Living (AAL) promotes the development and use of innovative technologies to allow older people to keep living in their own houses, rather than hospices or nursing homes. To this aim, AAL specifically designs intervention on homes to adapt them to different situations (health or disease), enhancing older people's autonomy, easing daily activities and guaranteeing safety conditions. So, new reliable devices and sensors systems capable to detect and monitor risk factor, medical condition, etc. are becoming very important.

One the most important medical needs is the inflammatory monitoring of Chronic Obstructive Pulmonary Disease (COPD) that is considered one of the leading causes of morbidity and mortality worldwide for elderly. Nowadays it's well appreciated the powerful potential of breath analysis for disease diagnostics and metabolic status monitoring. On one side, scientific research is devoting a lot of efforts in identifying markers of pathologies in exhaled breath by advanced analytical technologies, as gas chromatography combined with mass spectrometry (GC-MS), ion mobility spectrometry (IMS), proton transfer reaction mass spectrometry (PTR-MS), selected ion flow tube mass spectrometry (SIFTMS).

On the other side, instruments as Electronic Nose (EN) mainly based on semiconducting gas sensors (SGS), were in developing, offering an alternative to the above mentioned complex spectrometry techniques for a quick and easier breath analysis useful for qualitative analysis purposes and disease screening in population.

In this work, we try to combine an advanced analytical technique as GC-MS with semiconducting gas sensors (SGS) in order to study the ability of SGS to detect breath VOCs eluting from the gas chromatographic column. This approach looks to a future developing of miniaturized gas chromatographs based on gas sensors detector, acting as Point of Care system to be used by the elderly people at home for monitoring their health status.

#### #P180 - Production and characterization LKB, LMB and LCB borate glasses

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Glasses have been studied as potential luminescent dosimeters at high doses, especially in the last two decades. Borate glasses show high luminescence intensity compared to other glass matrices. However, they also have high hygroscopicity that is a major

disadvantage for practical dosimeters. Considering the intense research for materials that have favorable characteristics as optically stimulated luminescence dosimeters (OSL), different glass matrices give the opportunity of a systematic study. This work consisted of the evaluation of three distinct glass matrices (LKB, LMB and LCB) produced by rapid cooling. For each matrix, five subsets were produced with different compositions:  $\text{Li}_2\text{CO}_3 - \text{X} - \text{B}_2\text{O}_3$  [ $\text{X} = \text{K}_2\text{CO}_3$  (LKB),  $\text{MgO}$  (LMB) or  $\text{CaO}$  (LCB)], in order to determine the best composition in terms of OSL emission and moisture resistance. The hygroscopicity of the glasses was evaluated by two tests: against moisture and against water. After 40 days of exposition to moisture LKB glasses became opaque. The test of immersion in distilled water reinforced the finding that LKB matrix has a higher hygroscopicity compared to the LCB and LMB matrices. After one day the mass reduction was equal to 22.5% for LKB, 1.2% for LCB and 1.6% for LMB. We found a composition of LKB that emits 48% more intense OSL light than the basic matrix normally used for doping studies reported in the literature. The most sensitive subgroups of LMB and LCB presented a sensitivity that is much lower than the LKB. Therefore, LKB matrix, despite being more hygroscopic, it is also the most sensitive to radiation among the matrices that we studied.

#### #P181 - Intrinsic molecular-like luminescence from the surface of silica nanoparticles

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Amorphous silica plays a key role in the modern nano-science because of its appealing characteristics from both application and fundamental point of view. In addition to the wide transparency range, low conductivity and hardness, intimately related to the strong Si-O covalent bond, the reduction to nanoscale brings out new properties. One of the most relevant is the high photon emissivity in the UV-Visible range due to the formation of a large variety of luminescent defects favored by the high specific surface ( $\approx 100^2 \text{ m}^2/\text{g}$ ). A feature common to the photoluminescence bands usually observed in silica nanoparticles is the broad and structureless line-shape, this is accounted for by the homogeneous and inhomogeneous broadening. The first, related to the single defect, is mainly caused by the electron-phonon coupling and is therefore dependent on temperature; the second is related to the site-to-site non equivalence caused by the structural disorder in the short-range in comparison with the  $\text{SiO}_4$  tetrahedron size. An exception to these broad bands has been evidenced in a vacuum: a structured emission/excitation pattern is observed around 3.0-3.5 eV even at room temperature. This luminescence resembles that of a molecular-like system and is due to the coupling of an electronic transition with two localized modes of frequency  $1370 \text{ cm}^{-1}$  and  $360 \text{ cm}^{-1}$ . The understanding of this uncommon behavior in the field of the optical properties of defects in amorphous solids is the purpose of the present work. By using a tunable laser source and a time resolved detection, we carried out the investigation of the emission, excitation and decay properties of the vibronic progression as a function of temperature, thus deriving parameters useful to characterize the coupling strength. The results point out that on increasing temperature the intensity and the lifetime decrease due to the activation of a non-radiative channel from the excited state. Concurrently, the temperature dependence of the line-shape evidences the low coupling with non-localized modes of the matrix (Huang-Rhys factor  $S \approx 0.2$ ) and the poor influence of the inhomogeneous broadening. These findings outline that the silica surface can allocate luminescent defects almost disentangled from the basal network.

#### #P182 - Luminescence of isolated defects in nanostructured silica surface for small molecules detection

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The large variety of surface defects arising from the reduction to nanoscale is at the origin of the huge emissivity observed in  $\text{SiO}_2$  nanoparticles. Generally, broad and structureless emission bands characterize the UV-Visible spectral range, reflecting the amorphous matrix in which the defects are embedded. An exception is observed in a vacuum and consists of a structured photoluminescence, between 3.0 eV and 3.5 eV, whose sharp spectral features resemble those of a single molecule. This emission is due to the coupling of an electronic transition with two localized modes of frequency  $1370 \text{ cm}^{-1}$  and  $360 \text{ cm}^{-1}$ . Its quenching in air points out that the defects are allocated on the surface of the nanoparticles and strongly interact with the molecular species of the environment. The pronounced sensitivity to the atmosphere, in combination with the advantageous spectral features, is promising for the use of  $\text{SiO}_2$  nanoparticles as luminescent sensors. To this aim, the understanding of the fundamental mechanisms of the quenching is mandatory.

By using time resolved photoluminescence technique, we have carried out a detailed investigation of the effects on the spectral and decay properties of the structured emission induced by the interaction with  $\text{O}_2$  and  $\text{N}_2$ . Such interactions cause a photoluminescence quenching and a decrease of the lifetime ( $\tau$ ), the extent of which depends on the specific molecular species. Under  $\text{N}_2$ , the intensity quenching equals the  $\tau$  reduction in agreement with a collisional origin of the process. Under  $\text{O}_2$ , the quenching is larger than the  $\tau$  decrease, thus pointing out a combined collisional- and reaction-limited process. In both cases the phenomenon is reversible after restoring the vacuum, this indicates the weak (Van der Waals) interaction of the luminescent defects with  $\text{O}_2$  and  $\text{N}_2$ . All these findings highlight the possibility to discern the molecules by analyzing the spectroscopic variations of the structured emission, thus leading to the potential application of this system as probe of small molecules.

**#P183 - Development of a PECVD set up for nanomaterials production**

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The fabrication of nanomaterials, with controlled shapes and properties, requires a fine tailoring of the production methods. Among all, Plasma Enhanced Chemical Vapor Deposition (PECVD) has been recognized as the most promising approach for synthesizing nanostructures of various forms, since it is currently the only technique that allows size, alignment and orientation control of nanospecies. With this technique the growth of nanostructured material on a catalytic surface is enhanced by a plasma-surface interaction in a gas environment. The energy supplied by the plasma promotes the decomposition and activation of the reactant gases at the catalytic surface, thus allowing low-temperature processes ( $T \ll 1000^\circ\text{C}$ ) and more fine tuning of the synthesized material properties. In the last decades, PECVD has emerged as a key technique for the growth of carbon nanotubes (CNTs). The combination of extraordinary electric and mechanical properties offered by CNTs stimulates the research about their applications in fields ranging from electronics to sensing, from gas storage to optics. However, the production method is a crucial discriminating factor for displaying such properties. On this basis, due to its appealing features, the PECVD is the preferred approach for most CNTs fabrication needs.

Our work is aimed to the production of vertically aligned CNTs, which will serve as electron emitters of cold cathodes in X-ray sources. Here we show the first stage of the project, consisting of the development of an Electron Cyclotron Resonance - PECVD set up (ECR-PECVD). It is composed by a plasma chamber, where a  $\text{CH}_4$  and  $\text{H}_2$  mixture plasma is sustained by microwave cyclotronic resonance, and a process chamber, where the gas ions are accelerated by an electric field towards the catalytic substrate on which CNTs growth takes place. The characterization of the plasma generation and the preliminary results of the growth processes on catalytic supports are reported.

**#P184 - Multi-parametric study of the February-April 2013 paroxysmal phase of Mt. Etna New South-East crater**

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Between January 2011 and April 2013, Mt. Etna's eruptive activity consisted of episodic intra-crater strombolian explosions and paroxysms from Bocca Nuova, Voragine, and the New South-East (NSEC) summit craters, respectively. Eruptions from NSEC consisted of initial increasing strombolian activity and lava flow output, passing to short-lasting lava fountaining. In this study we present seismic, infrasound, radiometric, plume  $\text{SO}_2$  and HCl fluxes and geodetic data collected by the INGV monitoring system between May 2012 and April 2013. The multi-parametric approach enabled characterization of NSEC eruptive activity at both daily and monthly time scales and tracking of magma movement within Mt. Etna's plumbing system. While seismic, infrasound and radiometric signals give insight on the energy and features of the 13 paroxysms fed by NSEC,  $\text{SO}_2$  and halogen fluxes shed light on the likely mechanisms triggering the eruptive phenomena. GPS data provided clear evidence of pressurization of Mt. Etna's plumbing system from May 2012 to middle February 2013 and depressurization during the February-April 2013 eruptive activity. Taking into account geochemical data, we propose that the paroxysms' sequence represented the climax of a waxing-waning phase of degassing that had started as early as December 2012, and eventually ended in April 2013. Integration of the multidisciplinary observations suggests that the February-April 2013 eruptive activity reflects a phase of release of a volatile-rich batch of magma that had been stored in the shallow volcano plumbing system at least four months before, and with the majority of gas released between February and March 2013.

**#P185 - Thermal investigation and analysis on (dis)assembly and structural stability of chaperonins group I**

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Heat shock protein 60kDa is a molecular chaperone (GroEL human homolog) that assists protein folding in mitochondria (mtHsp60). It is synthesized in the cell cytoplasm as a higher molecular weight precursor form (p-mtHsp60) containing an N-terminal targeting sequence, that is cleaved after import into the mitochondrial matrix [1, 2]. In various pathological conditions (i.e., cancer and

chronic inflammatory diseases) Hsp60 can accumulate in the cytosol, with or without mitochondrial release concomitantly, so that in the cytosol the two types of 60 kDa chaperonin proteins, (mtHsp60 and its precursor naive form, p-mtHsp60) could coexist [3]. Despite the plethora of studies on the mechanism of Hsp60's function, especially in prokaryotes, fundamental issues still remain unexplored. Key questions still unanswered pertain to the differences in structure-function features that might exist between the well-studied prokaryotic GroEL and the largely unexplored eukaryotic Hsp60 proteins. Moreover, studies on human Hsp60 structure and oligomeric state in vitro could help to validate its role in physiological or pathological cases. In order to pursue this goal, High-sensitivity Nano Differential Scanning Calorimetry (Nano-DSC), Nano Isothermal Titration Calorimetry (Nano-ITC) and High Performance Liquid Chromatography (HPLC) were applied for the first time to study the (dis)assembly, structural and thermal stability of chaperonins group I. Complementary Circular Dichroism (CD) measurements were done to follow the change in the secondary structure due to unfolding. We found a more versatility and flexibility of eukaryotic (particularly mtHsp60) proteins than prokaryotic, suggesting that subunit flexibility should be closely related to the evolutionary history of a complex.

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### #P186 - Novel microfluidic centrifugal mixing device for small-angle X-ray scattering

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The high-brilliance beamline P12 is located at the PETRAIII storage ring (DESY, Hamburg) and it is dedicated to biological small-angle X-ray scattering (SAXS). P12 possesses a versatile and flexible sample environment that caters for diverse experimental needs to study macromolecular solutions. In addition to a robotic sample changer for standard SAXS experiments, we developed a novel microfluidic centrifugal mixing device (SAXS disc) to explore multiple equilibrium conditions while optimizing the sample consumption.

The SAXS disc is dedicated to high-throughput screening experiments and offers the handling and mixing of microliter quantities of sample. The disc is divided into identical and independent sextants that each constitutes an individual sample screen. Each sextant has three small reservoirs for depositing solutions: 2  $\mu$ l of sample, 3  $\mu$ l of mixing buffer and 3  $\mu$ l of screening buffer. Once the samples and buffers have been loaded onto their respective reservoirs using standard pipetting, the disc is loaded into a centrifuge device that spins the disc with a pre-programmed rotation speed pattern mixing the sample the buffer and the screen in precise ratios.

Although other microfluidic systems for SAXS are effectively miniaturized, the accessory components often required to control and operate the devices (pumps, valves, electronics, pneumatics, etc.) can be very bulky. SAXS disc is a centrifugal force driven microfluidic screening disc for solution SAXS measurements and forgoes the need for any external pump or valve attachments during SAXS data collection (Ducrée et al., 2007). Automatic alignment with the X-ray beam is under development to offer a user-friendly setup. Here we present a typical application of the SAXS disc to the study of a multiple equilibria phenomenon such as the unfolding of ribonuclease A as a function of urea content and a screening experiment testing the effect of salt concentration on inter-particle interactions in protein solutions.

These examples show that for high-throughput screening of solution additives, this microfluidic device offers an attractive alternative to standard SAXS data collection strategies.

### #P187 - Langevin theory of many-body systems coupled to non-equilibrium environments

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The generalized Langevin equations for many probe particles weakly interacting with a driven environment is derived by applying non-equilibrium linear response theory. When the driving is off, the theory correctly reproduces the equilibrium properties of the system, i.e. it fulfills the FDT and conforms to Onsager's regression principle relating the fluctuations of statistical forces to the memory kernel. Instead, in the presence of driving, we quantify in terms of both excess dynamical activity and probability currents the breaking of the fluctuation-dissipation theorem and reciprocal relations. The latter results in the lack of the action-reaction principle for the environment-mediated interactions. We test our findings with numerical simulations of active and driven particles.

### #P188 - Rotational and translational diffusion in an interacting active dumbbell system

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Active matter is characterized by the continuous partial conversion of internal energy into work. Some examples, at different scales, are the bacterial colonies, algae suspensions, bird flocks and schools of fish, but also colloidal particles being self-propelled artificially, for example, by surface treatment. All these systems live, or function, in conditions far from thermodynamic equilibrium and pose challenging questions to non-equilibrium statistical mechanics. The dynamical properties of an active system are significantly affected by self-propulsion. In particular, the diffusive properties are widely studied experimentally, either for the active particles themselves, or for passive tracers immersed in the active bath. I will consider here a two-dimensional system of active dumbbells, diatomic molecules formed by two spherical colloids and linked by a spring, with excluded volume interactions and immersed in an implicit solvent modeled by the Langevin equation. The activity is added as a constant force acting along the main axis of the dumbbell. The model can be intended as a very simplified version of natural swimmers, such as bacteria. I will focus in this talk on the translational and rotational properties of this system in a regime without phase separation, so in an homogeneous phase, showing that there are many different emerging properties due to the active force. In particular, four different regimes for the translational and angular mean square displacement can be retrieved, with a dependence of the diffusion coefficient from the temperature, activity and density. We find, for example, that for sufficiently high activity, the rotational diffusion is enhanced from increasing density, due to large-scale fluctuations, which is different from what usually happens in passive colloidal systems[1]. I will also show how the distribution functions of the displacement, especially at strong activity, deviates from the gaussian behavior at different typical timescales[2].

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#### #P189 - Negative ion source for nuclear fusion reactor

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The thermonuclear fusion reactor ITER will be heated by injection of a fast neutral beam (up to 1 MeV) generated by acceleration and neutralization of negative ions.

The negative ion source used for this purpose consists of driver volumes where radio-frequency power is inductively coupled to the plasma electrons and an expansion chamber containing a magnetic filter. At the end of the expansion region, the extraction consists of three different grids. The first Plasma Grid (PG) is a caesiated molybdenum surface which allows a large production of surface negative ions by neutral and positive ion conversion.

In this work, the self-consistent transport of electron, positive ions and  $H^-$  ions through the magnetic filter and in the extraction region of this source has been modelled by means of a two-dimensional Particle-in-Cell simulation. Results show the importance of the asymmetry created by the magnetic filter and of the potential bias of the PG in the maximization of the negative ion to electron extracted current ratio.

#### #P190 - Model and Experiment of Microwave-Plasma Interaction in MWPECVD

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Cutoff of radio communications during spacecraft atmospheric reentry and electromagnetic absorption of plasma plume thruster during satellite communication are two examples of wave-plasma interaction.

In this work, we simulate the plasma/electromagnetic 2.45 GHz wave interaction performed in *ad hoc* experiment using a microwave plasma enhanced chemical vapour deposition (MWPECVD) apparatus. Preliminary experimental studies have proved the presence of electromagnetic interaction observing fluctuations of reflected wave signals. In order to explain the experimental results we have implemented a model able to provide information about this fluctuation. The model concerns the discretization of the plasma volume in different slides. Each slide is characterized by a discrete value of the complex relative permittivity. At each slide interface the model estimates the transmitted and the reflected wave considering the 2.45 GHz wave impinging on the top of plasma volume. The simulations allow calculating the total reflection coefficient for different electromagnetic interactions due to  $H_2$ ,  $H_2/CH_4$ , and  $H_2/CH_4/N_2$  plasmas. This coefficient assesses the reflected signal fluctuations and plasma impedance variations representing the mismatch due to



the microwave interaction. Future improvements of the proposed model will include a self-consistent model of the plasma-gas phase able to correlate the reflected power with the electron temperature/kinetics of the plasma.

### #P191 - Quantum Dot Intermediate Band Solar Cells: Role of Al-based extended 2D states in photocarrier extraction and trapping

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Intermediate Band Solar Cells (IBSC) are an innovative concept of photovoltaic system with a theoretically predicted increased efficiency with respect to the Shockley-Queisser limit of single junction solar cell. Despite of the high potentialities of this theory, its practical applications are limited by the materials which can be effectively employed to get the required band profile. The most studied system so far consists of InAs Quantum Dots (QDs) self organized in a GaAs matrix [1-2], a system limited by the dominance of carrier thermal escape at room temperature induced by the related energy band profiling [3-4]. Further achievements within the IBSC concept are expected by the addition of Al both, in the GaAs barrier and in the InAs QD coverage [5-7]. However, QD self assembly via Stranski-Krastanov growth mode is widely known to be highly sensitive towards strain and surface conditions which are further complicated when ternary or quaternary compounds are used, because of the different atomic size and surface mobility of the group III adatoms.

In this work we present the study of an IBSC structure consisting of an AlGaAs barrier for QDs which were grown following a multistep procedure with a submonolayer Al-rich template, providing suitable conditions for strain field limitation and uniform QD organization. The optical role of this template with respect to device operation has been deeply investigated by means of different cw and modulation spectroscopy techniques, along with temperature studies of the photocurrent spectral generation by the application of an additional low energy pumping beam and of an external bias, showing the occurrence of carrier thermal transferring and interlevel filling processes between this state and the QD related energy positions. Further engineering on such a state and on its relationship with 3D confined QD states represents a promising way to extend IBSC design flexibility and to improve their efficiency.

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### #P192 - Ion irradiation of AZO thin films for flexible electronics

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Aluminum doped Zinc oxide (AZO) is a promising transparent conductor for solar cell, display and touch-screen technologies. AZO resistivity is typically improved by thermal annealing, not applicable to plastic substrates. Here we present a non-thermal route to improve the electrical and structural properties without deteriorating the optical ones, by using O<sup>+</sup> or Ar<sup>+</sup> ion beams (30 - 350 keV, 3x10<sup>15</sup> - 3x10<sup>16</sup> ions/cm<sup>2</sup>) on AZO deposited on glass and polyethylene naphthalate (PEN). X-Ray Diffraction, optical absorption, electrical measurements, Rutherford Backscattering Spectrometry and Atomic Force Microscopy evidenced an increase of the crystalline grain size and a complete relief of the lattice strain upon ion beam irradiation. Indeed, the resistivity of thin AZO films irradiated at room temperature decreased of two orders of magnitude, similarly to a thermal annealing at 400 °C. We showed that the improvement of the electrical properties does not simply depend on the strain or polycrystalline domain size, as often stated in the literature. The same process was successfully applied to AZO deposited on plastic substrate, so obtaining a flexible, transparent and conducting thin layer on plastic with not thermal budget.

### #P193 - Isotropic emulsion in a liquid crystal under shear

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#### EVALUATION OF GAMMA-RAY AND NEUTRON FLUXES IN A NEUTRON IRRADIATOR USED FOR RAD-HARD ELECTRONIC COMPONENTS TESTING

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#### ABSTRACT

An irradiator with four Am-Be neutron sources (activity 111 GBq each) was used for testing electronic RAD-HARD components developed for space application [1]. For this goal, an essential requirement to be met is the knowledge with sufficient precision of neutron and gamma-ray fluxes in the irradiation channel where the components are put for the test. For this goal, an experimental measurement activity was started to validate also Monte Carlo simulation results, obtained with application of MCNP5 code.

As regards gamma-ray flux, we considered separately two gamma-ray contributions: the first one, at 60 keV energy, associated with the decay of the <sup>241</sup>Am, and the second one, at 2.2 MeV, due to the radiative capture of neutrons in the biological shield (water) surrounding the neutron sources. Experimental measurements were realized with TLD700 dosimeters in two different configurations: TLD "naked" to measure the dose of the total gamma irradiation field, and TLD put inside a lead shield to determine (for difference) 60 keV gamma-ray contribution. The dimensions of used dosimeters, very small, allowed an accurate dose behaviour determination. For the TLD calibration, we exposed them to well-know doses values at the <sup>60</sup>Co irradiator named IGS3, situated in the Department of the University of Palermo.

As regards the evaluation of the neutron radiation field, experimental measurements were realized both by neutron activation with gold foils (nude and cadmium covered) and with thermoluminescent dosimeters (TLD600 and TLD700). Results have been compared with the ones obtained by a Monte Carlo (MCNP) simulation performed adopting a model of the irradiator previously validated [2].

The comparison between the experimental data and those obtained performing a Monte Carlo simulation allowed the determination of both neutron (thermal) and gamma field in several points inside the irradiation channel and, in particular, in those positions more used to the realization of irradiation tests.

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#### #P195 - Plasma techniques for the treatment of volatile organic compounds

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Among all the air pollutants emitted into the atmosphere, volatile organic compounds (VOCs) should be carefully considered, since chronic exposure by inhalation can negatively affect human health. In spite of increasingly stringent emission limits, the waste sector still contributes up to 4% of VOC emissions. The biofilters used in the mechanical-biological treatment of waste are particularly sensitive to changes in the composition of the gaseous effluent and to unsteady airflow rates, since microorganisms require time to acclimatize. During transient conditions, the removal efficiency of biological technologies is limited. Consequently, an upstream device, which integrates the gas treatment to improve the performances of the biofilter, would be useful. In this framework, non-thermal plasmas (NTPs) offer interesting opportunities in the field of air-cleaning systems [1, 2]. Atmospheric NTPs are an environmentally-friendly and promising technique for removing several air pollutants. The energy of the electric field is mainly transferred to the electrons, which therefore have a much higher temperature than the gas molecules. As a consequence, electron dissociation processes promote a "high energy" chemistry at room temperature, which fosters the dissociation of very stable molecules.

The aim of this research is to investigate the effect of NTPs on mixtures of VOCs representing real emissions from specific industrial and waste treatment processes that use biofiltration or biotrickling filtration for air pollution control

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**#P196 - Reforming of CO<sub>2</sub> and CH<sub>4</sub> by a nanosecond pulsed discharge at atmospheric pressure**

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The conversion of the main greenhouse gases, CO<sub>2</sub> and CH<sub>4</sub>, into value added chemicals and liquid fuels is considered as one of the main challenges at the present time. If the process is sustained by green energy, solar energy is then stored in chemical energy, producing the so called 'solar fuels' [1]. Conventional thermal methods suffer many drawbacks. Techniques based on cold plasmas are a promising option, since they operate at low temperature, thus reducing thermal losses. In addition, plasma based systems are characterized by low inertia, and therefore are inherently quick-start devices, suitable for the consumption of excess renewable energy.

Dielectric Barrier Discharges, DBD, have long been investigated, due to their simplicity and reliability. When CO<sub>2</sub> and CH<sub>4</sub> are the feed gases, DBD produce syngas and light hydrocarbons, but also liquid oxygenates [2] and liquid hydrocarbons [3]. Unfortunately, both the conversion rate and the global energy efficiency are low. To overcome these limitations, the synergy between plasma and catalysis is actively explored at the present. A complementary route is to attempt different discharge configurations. Nanosecond pulsed discharge (NPD) are characterized by higher mean electron energies. Therefore one presumes higher dissociation rates and eventually higher conversion values.

Here we report on results obtained by using a nanosecond pulsed discharge to activate a mixture of CH<sub>4</sub> and CO<sub>2</sub>. With respect to DBD, we observe a significant increase of the reactant conversion and a different branching ratio. In particular, NPD increases the selectivity towards solid carbon and light gaseous chemicals (H<sub>2</sub>, CO, C<sub>2</sub>H<sub>2</sub>), at the expense of liquid hydrocarbons and oxygenated compounds.

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**#P197 - RF plasma-jets at atmospheric pressure: a source of ROS to investigate oxidation processes**

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Atmospheric pressure plasma jets allow the generation of reactive oxygen species (ROS), such as OH(<sup>2</sup>P<sub>3/2</sub>), O(<sup>3</sup>P) and O<sub>2</sub>(<sup>3</sup>S<sub>g</sub>) radicals, and can be utilized to investigate radical-initiated oxidation processes. By using a RF plasma jet of He/O<sub>2</sub>, we studied the reactivity of naphthalene with oxygen species and the role of oxidative reactions in the growth of polycyclic aromatic hydrocarbons [1].

In the present work, we have used a plasma jet of He/H<sub>2</sub>O to investigate the oxidation of fatty acid methyl esters (FAME). We have exploited laser induced fluorescence [2] to measure the OH concentration in the plasma plume impinging on the FAME target. OH radicals produced in the discharge trigger the oxidation of unsaturated FAME. A systematic analysis of the oxidation products as a function of the flux of OH radicals will be presented.

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**#P198 - Metal-free, Iron and Manganese Phthalocyanine: a comparison between Valence Band Photoelectron Spectra**

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Phthalocyanines (Pcs) are a class of widely studied molecules due to the possibility to deposit them in molecular film and obtain molecular materials with tunable properties and a variety of technological applications. Among all different kind of Pcs, transition metal Pcs (TMPcs) are particularly interesting because they can be used as organic semiconductor in molecular electronic but also

as spin filter in spintronics [1, 2]. The 3d states are responsible for TMPcs molecular magnetic and conduction properties and their occupancy is reflected on the behavior of TMPcs valence band (VB) region.

In this work we present a photoemission spectroscopy (PES) investigation on the VB region of two different TMPcs, iron and manganese phthalocyanines (FePc and MnPc, respectively), compared with the VB of metal-free phthalocyanine (H2Pc), in order to elucidate these important states and to clarify the influence of the central metal atoms on the Pcs VB structures.

PES measurements were performed on the molecules in gas phase and as molecular films, with different photon energies that, together with density functional theory (DFT) calculations, allow us to identify and isolate the different atomic contributions to the valence spectral peaks [3]. We show that the molecular structure of a TMPc originates from the hybridization (orbital combination) of the N and C with the central metal atom. By comparing the low energy region of the FePc VB film with that measured in gas phase, we show that the two peaks, HOMO and HOMO-1 (Highest Occupied Molecular Orbital) distinguishable in gas phase, are merged in one broader peak in the film, due to intermolecular interactions in the adsorbate case. Moreover, from the comparison between, FePc, MnPc and H2Pc gas phase VB spectra, we conclude that FePc and H2Pc HOMO related peaks coincide with MnPc HOMO-1 peak, because all these features are due to C2p contributions.

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#### #P199 - Dynamics of coherence and quantum correlations for continuous variable systems interacting with classical environment

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We address the dynamics of the decoherence process of a continuous variable system interacting with a classical fluctuating environment. As a paradigmatic example, we analyze the case of a quantum harmonic oscillator prepared in a nonclassical state, focusing on the relevant role played by the correlations of the environment that rule the decoherence dynamics. Also, we investigate the influence of the stochastic environment on the time evolution of quantum correlations of a bipartite system.

#### #P200 - Spectral and decay properties of defects related luminescence in sintered silica nanoparticles

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Bulk silica is a material of choice in optics and electronics because of its exceptional properties (transmission and insulating power). Its reduction to nanoscale introduces peculiarities due to a network rearrangement, in particular the high specific surface ( $\sim 10^2 \text{ m}^2/\text{g}$ ) favors the formation of a wide variety of surface defects which confer functional properties such as the high emissivity. Several studies have addressed the inverse process, from nanoparticles to bulk transparent glass, induced by solid-phase sintering activated by thermal treatments at temperatures ( $\sim 1000 \text{ }^\circ\text{C}$ ) far below the melting point. IR and microscopy techniques have clarified the structural properties of the sintered material in the medium and long range order pointing out the similarities with the bulk silica. As concerns the optical properties related to the short range order it is known that this material exhibits a bright visible emission under UV excitation, this feature being associated with point defects peculiar to sintered material. The study of the spectral and decay properties of the luminescence bands is therefore crucial both to identify the defect structure and to probe the surrounding silica network.

In this work we have investigated a transparent sample produced by the sintering (thermal treatment at  $1000 \text{ }^\circ\text{C}$  for 272 hours) of silica nanoparticles with an average diameter of 14 nm. The use of time resolved luminescence spectroscopy and a tunable laser source has allowed us to single out three emissions centered around 1.9 eV, 2.4 eV and 3.4 eV. The excitation spectra evidence bell shaped bands consistent with transitions between localized defects states. We have studied the luminescence intensity and the lifetime in the temperature range from 300 K down to 10 K, thus evidencing the competition between radiative and non-radiative processes in the optical cycle. On the basis of the observed features, these emissions cannot be associated with well-known silica defects, neither in bulk samples nor in nanoparticles.

#### #P201 - Interference and Thermoelectric effects in tunnel-coupled quantum Hall liquids

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We study thermal transport between two tunnel-coupled quantum Hall systems (QHS) with different filling factors belonging to the Laughlin sequence. We consider both charge and heat currents due to a temperature gradient between the two QHS for a generic tunneling region. Specifying to the case of multiple quantum point contacts (QPCs) geometry, we demonstrate that both charge and heat currents present oscillating behaviors due to interference paths for electrons and holes. In particular, the sign of the charge current can be changed acting on the distance between the QPCs. We analyze these features in the non interacting case (integer fillings) and in presence of interactions, considering tunneling of electrons between different fractional and integer QHS. In this case we also show that large heat rectification effects can be achieved. We find that a multiple QPC geometry leads to larger rectification effects in comparison to the case of single QPC. This is linked to the presence of interference pattern in the heat current signal.

#### **#P202 - Hall-MHD and hybrid Vlasov-Maxwell simulations of kinetic Alfvén waves within phase-mixing process**

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In the range of proton kinetic scales and even down to typical electron kinetic scales, many solar-wind observational analyses, theoretical works and numerical simulations suggest that the so-called kinetic Alfvén waves (KAWs) can play an important role in the mechanisms of turbulent energy dissipation and heating. Mathematically, KAWs are a wave solution of the two-fluid dispersion relation, in propagation quasi-perpendicular to a background magnetic field. They can be considered as the continuation of the magnetohydrodynamic (MHD) Alfvén mode at scales comparable to the ion skin depth, and/or the ion Larmor radius.

Considering their high characteristic angles of propagation, KAWs have been invoked to explain the excess of perpendicular energy in observational data of the solar-wind magnetic field. So far, the physical mechanisms responsible for the production of the KAWs are still on debate. Since phase-mixing can generate quasi-perpendicular Alfvén fluctuations, in this work we investigate whether it can trigger KAWs excitation. To this purpose, we need to study this physical process in a range of scale that goes at least from the smallest scales of MHD to a fraction of the ion skin depth, in linear and nonlinear regimes of wave propagation. To resolve the kinetic scales, we use the low noise hybrid Vlasov-Maxwell (HVM) code (Valentini et al., 2007) and an Hall-MHD code to control the smallest MHD scales. For the linear regime, we present some physical properties of the perturbations produced after the Alfvén speed shear, which are in good agreement with those discussed by, e.g., Vasconez et al., in 2014 (and references therein).

#### **#P203 - Energetic neutral particle beam interaction with thermonuclear plasmas: from present day experiments to reactor parameters**

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The magnetic confinement of thermonuclear plasmas is a possible way to exploit fusion reactions from light nuclei in order to produce electricity. In a future fusion reactor the plasma must reach temperatures of tens of keV to produce enough fusion reactions. Due to the decrease of plasma resistivity with temperature, in Tokamak magnetic configuration the ohmic heating generated by the induction of a current in the plasma cannot sustain by itself a thermonuclear plasma discharge. To reach fusion relevant temperatures, auxiliary heating systems are used in present day experiments. The injection of energetic (of the order of 100 keV) H/D neutral particles in the plasma (by Neutral Beam Injectors NBIs) is one of the most used techniques to heat the plasma, since early 1970s [1]. NBI led to significant breakthroughs like the discovery of plasma high-confinement mode – H-mode – in 1982 at ASDEX Tokamak [2], a high performing plasma scenario which represents the basis for present day experiments and future fusion reactors. During 1990s experiments equipped with several MW of NBI power were the first to produce a significant amount of energy from fusion reactions. Basic physics phenomena are involved in the interaction between the neutral energetic particles from the beam and the plasma. These include beam ionization by collisions with plasma electrons and ions and by charge exchange processes, and the thermalization of the newly born fast ions in the background plasma by Coulomb collisions (“slowing down” process).

In this contribution we investigate the interaction between energetic beam particles and the plasma and in particular how the choice of beam parameters influences the above-mentioned scenarios. NBI is in fact not only a source of heating: it is a particle source and depending on the injection direction it can induce plasma momentum and drive a current in the plasma helping to sustain a desired current density profile. Injection geometry and energy are then the crucial parameters which set the penetration of the beam in the plasma and the capability of driving beneficial non-inductive currents.

With the planned increase of plasma volume and density in future fusion reactors with respect to present day experiments, the energy of neutral beams must be increased up to 1 MeV in order to ensure an efficient plasma core heating. The present work describes the effect of the increase of the NBI energy on beam-plasma interactions such as driven flow, current and plasma heating and discusses related issues such as the “shine-through” problem, which consists in the not-full absorption of the high energy beam from the plasma and the consequent harm to the device first wall.

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**#P204 - Energy concentration factor for collective excitations in bi-component magnonic crystals**

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A quantitative estimation of the degree of localization of collective modes in binary magnonic crystals is given. This is accomplished by recalling the definition of the energy concentration factor in a photonic crystal written in terms of the spatially varying electric field and of the periodic non-uniform permittivity [1]. The binary magnonic crystals have periodicities in the nanometric range and are composed by a periodic arrangement of cylindrical cobalt (Co) nanodots completely embedded into a permalloy (Py, Ni<sub>80</sub>Fe<sub>20</sub>) continuous thin magnetic film. The lattice constant of the two-dimensional binary magnonic crystal is 600 nm and the external magnetic field is applied along the  $y$  direction in the plane of the system. The energy concentration factor for periodic binary magnonic crystals is defined as the ratio between the internal energy stored by the collective mode in the region having the higher internal field and its total energy [2]. The collective mode dynamical properties in a two-dimensional periodic and binary magnonic crystal are expressed in terms of the oscillating periodic dynamic magnetization which is a function of the Bloch wave vector. It has been found that the magnitude of the energy concentration factor strictly depends on the contrast between the saturation magnetizations of Co and Py. Analytical forms of the energy concentration factor are derived both at the centre of the Brillouin zone and as a function of the Bloch wave vector. As an example, a numerical estimation at the centre of the Brillouin zone at an external field of intensity  $H = 500$  Oe gives a value of only 9% due to the weak variation of the internal field. The computation of the energy localization factor for different geometries and for different values of the Bloch wave vectors is also given and a quantitative comparison among the several cases is presented.

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Gallo Salvatore	#601	Biomedical Applications	2 Oct
Galvanetto Nicola	#372	Electronic and optical properties of low dimensional systems I	1 Oct
Gambarini Grazia	#513	Dosimetry	2 Oct
Gambassi Andrea	#574	Out of Equilibrium Statistical Mechanics II	2 Oct
Gambino Marianna	#123	Sustainable Nanotechnologies II	29 Sept
Garlaschelli Diego	#490	Econophysics	2 Oct
Gentile Paola	#289	Topological Insulators	30 Sept
Gentilini Silvia	#297	Non Linear Optics	30 Sept
Gerbi Andrea	#371	Electronic and optical properties of low dimensional systems I	1 Oct
Ghiringhelli Giacomo	#331	New physics with ultrashort light and x-ray pulses I	1 Oct
Giacomazzi Luigi	#453	Advanced Optical Materials II	1 Oct
Giacometti Achille	#381	Soft Matter I	1 Oct
Giacopetti Laura	#015	Cultural Heritage	28 Sept
Gianfrani Livio	#532	Metrology	2 Oct
Giannetti Claudio	#036	Cuprates and Mechanisms for Superconductivity	28 Sept
Giansanti Andrea	#162	Computational Biophysics III	29 Sept
Giazotto Francesco	#426	Quantum thermodynamics and quantum technologies 1	1 Oct
Gigli Giuseppe	#207	Sustainable Nanotechnologies III	29 Sept
Ginelli Francesco	#248	Statistical Mechanics of Active Matter	30 Sept
Giorgetti Alejandro	#004	Computational Biophysics I	28 Sept
Giovannetti Gianluca	#223	2D emerging materials II	29 Sept
Girard Sylvain	#359	Advanced Optical Materials I	1 Oct
Gisselbrecht Mathieu	#326	New physics with ultrashort light and x-ray pulses I	1 Oct
Goldoni Guido	Goldoni #020	Simulations of Materials for ICT	28 Sept
Goletti Claudio	#116	Oxide Films and Interfaces	29 Sept



Gomez Rivas Jaime	#044	Optical feedback and metamaterials in mid-IR and THz	28 Sept
Gonnella Giuseppe	#246	Statistical Mechanics of Active Matter	30 Sept
González Rivera José	#054	Sustainable Nanotechnologies I	28 Sept
Goold John	#425	Quantum thermodynamics and quantum technologies 1	1 Oct
Gottfried J. Michael	#433	Organic on Substrates III	1 Oct
Gradenigo Giacomo	#401	Transport and anomalous dynamics	1 Oct
Gradzielski Michael	#048	Sustainable Nanotechnologies I	28 Sept
Grasso Daniela	#024	Plasma Physics I	28 Sept
Grazianetti Carlo	#141	2D emerging materials I	29 Sept
Greco Giorgia	#628	Synchrotron radiation and material science II	2 Oct
Gregoratti Luca	#559	Advanced materials for energy applications III	2 Oct
Grifoni Milena	#482	Out of Equilibrium Statistical Mechanics I	2 Oct
Guarcello Claudio	#279	Thin films, Devices, Weak Superconductivity and Applications	30 Sept
Guarino Anita	#039	Cuprates and Mechanisms for Superconductivity	28 Sept
Gubbiotti Gianluca	#267	Magnetism and Spin related Phenomena III	30 Sept
Gueli Anna M.	#602	Biomedical Applications	2 Oct
Guerin Stephane	#333	Quantum Optics and Coherent Manipulation	1 Oct
Guidoni Leonardo	#071	Computational Biophysics II	29 Sept
Guizal Brahim	#128	Quantum Fluctuations and Casimir Forces	29 Sept
Gupta Anupam	#466	Soft Matter II	1 Oct
Guzzi Rita	#242	Molecular Biophysics I	30 Sept
Hedayat Zadeh Roodsari Hamoon	#192	Magnetism and Spin related phenomena IV	29 Sept
Heun Stefan	#367	Electronic and optical properties of low dimensional systems I	1 Oct
Hofmann Stephan	#439	Nanomaterials and Nanotechnology: carbon nanotubes	1 Oct
iacobucci stefano	#554	Synchrotron radiation and material science I	2 Oct
Iannotta Salvatore	#525	Diamond-based substrates and Memristors for Brain sensing	2 Oct
ienco andrea	#542	Electronical and optical properties of low dimensional systems III	2 Oct
Imparato Alberto	#572	Out of Equilibrium Statistical Mechanics II	2 Oct
Iori Giulia	#492	Econophysics	2 Oct
Irvine John T. S.	#118	Sustainable Nanotechnologies II	29 Sept
Joyce Michael	#077	Interdisciplinary statistical physics.	29 Sept
Kamran Muhammad	#280	Thin films, Devices, Weak Superconductivity and Applications	30 Sept
Kantorovich Sofia	#383	Soft Matter I	1 Oct
Karner Carina	#250	Statistical Mechanics of Active Matter	30 Sept
Keilmann Fritz	#055	Nanophotonics I	28 Sept

Kertesz Janos	#581	Complex Networks in Economy, Biology, ...	2 Oct
Kimberg Victor	#419	New physics with ultrashort light and x-ray pulses II	1 Oct
Kob Walter	#376	Soft Matter I	1 Oct
Kolmakov Andrei	#385	Advanced materials for energy applications I	1 Oct
La Magna Antonino	#229	2D emerging materials II	29 Sept
Laio Alessandro	#070	Computational Biophysics II	29 Sept
Lamia Debora	#508	Dosimetry	2 Oct
Lamporesi Giacomo	#314	Correlated electrons and cold atoms	1 Oct
Lanzani Guglielmo	#438	Nanomaterials and Nanotechnology: carbon nanotubes	1 Oct
Larciprete Rosanna	#611	Nanomaterials and Nanotechnology: Graphene	2 Oct
Lattanzi Gianluca	#156	Computational Biophysics III	29 Sept
Lazzeri Luigi	#510	Dosimetry	2 Oct
Leanza Renata	#507	Dosimetry	2 Oct
Leggio Bruno	#335	Quantum Optics and Coherent Manipulation	1 Oct
Leo Antonio	#281	Thin films, Devices, Weak Superconductivity and Applications	30 Sept
Leporatti Stefano	#571	Molecular Biophysics II	2 Oct
Lepore Maria	#570	Molecular Biophysics II	2 Oct
Lepri Stefano	#399	Transport and anomalous dynamics	1 Oct
Lettieri Stefano	#355	Gas Sensors and Biosensors for Health and Wealth	1 Oct
Leuzzi Luca	#081	Interdisciplinary statistical physics.	29 Sept
Libertino Sebania	#198	Optical bio-sensing	29 Sept
Liotta Leonarda	#122	Sustainable Nanotechnologies II	29 Sept
Lippiello Eugenio	#415	Geophysics	1 Oct
Liseykina Tatyana	#266	Plasma Physics IV	30 Sept
Lisi Simone	#434	Organic on Substrates III	1 Oct
Listorti Andrea	#210	Sustainable Nanotechnologies III	29 Sept
Livi Roberto	#608	Complexity in the brain	2 Oct
Lizzit Silvano	#551	Synchrotron radiation and material science I	2 Oct
Lo Cicero Matteo	#346	Organic on Substrates I	1 Oct
Lo Faro Maria Josè	#447	Advanced Optical Materials II	1 Oct
Lo Faro Massimiliano	#121	Sustainable Nanotechnologies II	29 Sept
Locatelli Emanuele	#167	Diffusion and reaction in complex systems	29 Sept
Lodari Mario	#549	Electronical and optical properties of low dimensional systems III	2 Oct
Lombardi Floriana	#275	Thin films, Devices, Weak Superconductivity and Applications	30 Sept
Lombardo Salvatore	#460	Electronic and optical properties of low dimensional systems II	1 Oct

Lorenzi Roberto	#448	Advanced Optical Materials II	1 Oct
Lorenzo Salvatore	#428	Quantum thermodynamics and quantum technologies 1	1 Oct
Lubritto Carmine	#014	Cultural Heritage	28 Sept
Lubritto Carmine	#472	Advanced materials for energy applications II	1 Oct
Luca Labate	#180	Plasma Physics III	29 Sept
Luetkens Hubertus	#104	Iron Based Superconductors	29 Sept
Lullo Giuseppe	#527	Diamond-based substrates and Memristors for Brain sensing	2 Oct
Lupi Stefano	#284	Topological Insulators	30 Sept
Macrì Vincenzo	#486	Out of Equilibrium Statistical Mechanics I	2 Oct
Magazzù Luca	#578	Out of Equilibrium Statistical Mechanics II	2 Oct
Maiolo Luca	#444	Nanomaterials and Nanotechnology: carbon nanotubes	1 Oct
Maiorano Vincenzo	#437	Organic on Substrates II	1 Oct
Malagò Perla	#268	Magnetism and Spin related Phenomena III	30 Sept
Malara Angela	#361	Advanced Optical Materials I	1 Oct
Malara Pietro	#540	Fiber and Miniaturized Optical Sensors	2 Oct
Mallocci Giuliano	#006	Computational Biophysics I	28 Sept
Malvestuto Marco	#422	New physics with ultrashort light and x-ray pulses II	1 Oct
Mana Giovanni	#528	Metrology	2 Oct
Manera Maria Grazia	#620	Advanced optical characterization techniques	2 Oct
Manno Mauro	#076	Computational Biophysics II	29 Sept
Manno Mauro	#309	Biophysical Models I	1 Oct
Manno Mauro	#169	Diffusion and reaction in complex systems	29 Sept
Marangoni Marco	#349	Gas Sensors and Biosensors for Health and Wealth	1 Oct
Marcuzzi Matteo	#579	Out of Equilibrium Statistical Mechanics II	2 Oct
Mariani Carlo	#624	Synchrotron radiation and material science II	2 Oct
Marino Emanuele	#449	Advanced Optical Materials II	1 Oct
Marino Jamir	#576	Out of Equilibrium Statistical Mechanics II	2 Oct
Marotta Luca Marotta	#582	Complex Networks in Economy, Biology, ...	2 Oct
Marré Daniele	#111	Oxide Films and Interfaces	29 Sept
Marri Ivan	#298	Photonic and plasmonic materials and devices	30 Sept
Marrucci Lorenzo	#252	Light Manipulation	30 Sept
Marsi Marino	#552	Synchrotron radiation and material science I	2 Oct
Martelli Fausto	#406	Molecular liquids in equilibrium and non-equilibrium regimes	1 Oct
Martini Marco	#008	Cultural Heritage	28 Sept
Maruccio Giuseppe	#353	Gas Sensors and Biosensors for Health and Wealth	1 Oct

Massobrio Paolo	#605	Complexity in the brain	2 Oct
Mastria Rosanna	#214	Sustainable Nanotechnologies III	29 Sept
Mataloni Paolo	#514	Quantum thermodynamics and quantum technologies 2	2 Oct
Mattei Giovanni	#085	From nanoparticles to nanostructured surfaces	29 Sept
Mattoni Alessandro	#204	3d and 5d TM systems	29 Sept
Mauri Francesco	#610	Nanomaterials and Nanotechnology: Graphene	2 Oct
Mazzamuto Giacomo	#145	Nanophotonics II	29 Sept
Mazzarella Giovanni	#339	Quantum Optics and Coherent Manipulation	1 Oct
Mazzeo Marco	#621	Advanced optical characterization techniques	2 Oct
Meinardi Francesco	#360	Advanced Optical Materials I	1 Oct
Memmolo Pasquale	#456	Electronic and optical properties of low dimensional systems II	1 Oct
Merlone Andrea	#533	Metrology	2 Oct
Messina Fabrizio	#363	Advanced Optical Materials I	1 Oct
Messina Riccardo	#131	Quantum Fluctuations and Casimir Forces	29 Sept
Mezzapesa Francesco	#152	THz and Quantum Cascade Lasers	29 Sept
Miccio Lisa	#231	Optofluidics	29 Sept
Micheletti Cristian	#390	Biophysical Models II	1 Oct
Minola Matteo	#271	Magnetism and Spin related Phenomena III	30 Sept
Mio Antonio Massimiliano	#547	Electronical and optical properties of low dimensional systems III	2 Oct
Mirabella Salvo	#358	Gas Sensors and Biosensors for Health and Wealth	1 Oct
Miseikis Vaidotas	#134	2D emerging materials I	29 Sept
Modica Aurora	#012	Cultural Heritage	28 Sept
Molle Alessandro	#135	2D emerging materials I	29 Sept
Montalenti Francesco	#018	Simulations of Materials for ICT	28 Sept
Monteleone Giuseppe	#115	Oxide Films and Interfaces	29 Sept
Monticelli Marco	#598	Biomedical Applications	2 Oct
Moras Paolo	#270	Magnetism and Spin related Phenomena III	30 Sept
Moretti Marco	#200	3d and 5d TM systems	29 Sept
Moroni Matteo	#108	Iron Based Superconductors	29 Sept
Mosca Sara	#010	Cultural Heritage	28 Sept
mosca simona	#295	Non Linear Optics	30 Sept
Motta Mario	#318	Correlated electrons and cold atoms	1 Oct
Muzzi Luigi	#277	Thin films, Devices, Weak Superconductivity and Applications	30 Sept
Negro Matteo	#327	New physics with ultrashort light and x-ray pulses I	1 Oct
Nerattini Francesca	#073	Computational Biophysics II	29 Sept

Nevin Austin	#321	Imaging and non-destructive analysis	1 Oct
Nocente Massimo	#095	Plasma Physics II	29 Sept
Nocentini Sara	#256	Light Manipulation	30 Sept
Nuzzi Davide	#102	Magnetism and Spin related phenomena II	29 Sept
Olivero Paolo	#454	Electronic and optical properties of low dimensional systems II	1 Oct
Onida Giovanni	#019	Simulations of Materials for ICT	28 Sept
Orlandini Enzo	#462	Soft Matter II	1 Oct
Orlando Gianfranco	#068	Laser-Matter Interaction: from Atoms to Nano-Particles	28 Sept
Ortenzi Luciano	#205	3d and 5d TM systems	29 Sept
Pacilè Daniela	#224	2D emerging materials II	29 Sept
Pagano Roberto	#597	Biomedical Applications	2 Oct
Pagnani Andrea	#155	Computational Biophysics III	29 Sept
Paladino Elisabetta	#516	Quantum thermodynamics and quantum technologies 2	2 Oct
Palmer Richard E	#083	From nanoparticles to nanostructured surfaces	29 Sept
Panaccione Giancarlo	#099	Magnetism and Spin related phenomena II	29 Sept
Panzeca Salvatore	#512	Dosimetry	2 Oct
Paparo Domenico	#471	Advanced materials for energy applications II	1 Oct
Parente Vincenzo	#137	2D emerging materials I	29 Sept
Paris Eugenio	#041	Cuprates and Mechanisms for Superconductivity	28 Sept
Parisi Luca	#023	Simulations of Materials for ICT	28 Sept
Pasquarelli Alberto	#521	Diamond-based substrates and Memristors for Brain sensing	2 Oct
Pasquini Luca	#467	Advanced materials for energy applications II	1 Oct
Passoni Matteo	#091	Plasma Physics II	29 Sept
Pastore Mariachiara	#386	Advanced materials for energy applications I	1 Oct
Paternò Giuseppe	#564	Advanced materials for energy applications III	2 Oct
Patriarca Marco	#089	From nanoparticles to nanostructured surfaces	29 Sept
Pattelli Lorenzo	#146	Nanophotonics II	29 Sept
Paturzo Melania	#196	Optical bio-sensing	29 Sept
Pavesi Lorenzo	#299	Photonic and plasmonic materials and devices	30 Sept
Pedio Maddalena	#034	Magnetism and spin related phenomena I	28 Sept
Pedrinazzi Paolo	#375	Electronic and optical properties of low dimensional systems I	1 Oct
Pellicane Giuseppe	#404	Molecular liquids in equilibrium and non-equilibrium regimes	1 Oct
Pendolino Flavio	#613	Nanomaterials and Nanotechnology: Graphene	2 Oct
Peng Yingying	#038	Cuprates and Mechanisms for Superconductivity	28 Sept
Pennetta Cecilia	#500	Environmental Physics and Pollution	2 Oct

Peres Giovanni #179	Plasma Physics III	29 Sept
Pevere Federico #301	Photonic and plasmonic materials and devices	30 Sept
Pfeifer Thomas #325	New physics with ultrashort light and x-ray pulses I	1 Oct
Piazza Aurora #228	2D emerging materials II	29 Sept
Piazza Francesco #164	Diffusion and reaction in complex systems	29 Sept
Piccinin Simone #563	Advanced materials for energy applications III	2 Oct
Piccinini Massimo #362	Advanced Optical Materials I	1 Oct
Piccolo Federico #522	Diamond-based substrates and Memristors for Brain sensing	2 Oct
Picone Andrea #114	Oxide Films and Interfaces	29 Sept
Picozzi Silvia #201	3d and 5d TM systems	29 Sept
Pierantozzi Gian Marco #556	Synchrotron radiation and material science I	2 Oct
Pieri Pierbiagio #320	Correlated electrons and cold atoms	1 Oct
Pietralunga Silvia Maria #614	Nanomaterials and Nanotechnology: Graphene	2 Oct
Pini Roberto #612	Nanomaterials and Nanotechnology: Graphene	2 Oct
Pisignano Dario #142	Nanophotonics II	29 Sept
Pizzella Vittorio #595	Biomedical Applications	2 Oct
Pizzocaro Marco #530	Metrology	2 Oct
Plastina Francesco #515	Quantum thermodynamics and quantum technologies 2	2 Oct
Plastino Wolfango #498	Environmental Physics and Pollution	2 Oct
Ponzoni Luca #396	Biophysical Models II	1 Oct
Porzio Alberto #254	Light Manipulation	30 Sept
Potestio Raffaello #158	Computational Biophysics III	29 Sept
Prando Giacomo #109	Iron Based Superconductors	29 Sept
Prestipino Santi #407	Molecular liquids in equilibrium and non-equilibrium regimes	1 Oct
Principi Alessandro #616	Nanomaterials and Nanotechnology: Graphene	2 Oct
Privitera Vittorio #049	Sustainable Nanotechnologies I	28 Sept
Puccio Elena #583	Complex Networks in Economy, Biology, ...	2 Oct
Pucella Gianluca #261	Plasma Physics IV	30 Sept
Puglisi Giuseppe #413	Geophysics	1 Oct
Puglisi Rosaria Anna #220	Photovoltaic materials and devices	29 Sept
Pulci Olivia #455	Electronic and optical properties of low dimensional systems II	1 Oct
Putti Marina #105	Iron Based Superconductors	29 Sept
Raciti Rosario #543	Electronical and optical properties of low dimensional systems III	2 Oct
Rajendran Sai Kiran #338	Quantum Optics and Coherent Manipulation	1 Oct
Rapisarda Andrea #496	Econophysics	2 Oct

Ratto Gian Michele	#618	Advanced optical characterization techniques	2 Oct
Ratynskaia Svetlana	#182	Plasma Physics III	29 Sept
Ravaro Marco	#151	THz and Quantum Cascade Lasers	29 Sept
Ricciardi Carlo	#524	Diamond-based substrates and Memristors for Brain sensing	2 Oct
Ricciardi Iolanda	#294	Non Linear Optics	30 Sept
Rinaldi Christian	#100	Magnetism and Spin related phenomena II	29 Sept
Ripepe Maurizio	#412	Geophysics	1 Oct
RIPPA MASSIMO	#541	Fiber and Miniaturized Optical Sensors	2 Oct
Ritort Felix	#391	Biophysical Models II	1 Oct
Ritter Petra	#520	Diamond-based substrates and Memristors for Brain sensing	2 Oct
Rizi Vincenzo	#501	Environmental Physics and Pollution	2 Oct
Rizza Carlo	#046	Optical feedback and metamaterials in mid-IR and THz	28 Sept
Rizzo Aurora	#219	Photovoltaic materials and devices	29 Sept
Rizzuti Bruno	#074	Computational Biophysics II	29 Sept
Roddaro Stefano	#186	Magnetism and Spin related phenomena IV	29 Sept
Rogero Celia	#343	Organic on Substrates I	1 Oct
Roldan Rafael	#370	Electronic and optical properties of low dimensional systems I	1 Oct
Romé Massimiliano	#027	Plasma Physics I	28 Sept
Romeo Francesco	#287	Topological Insulators	30 Sept
Ronda Luca	#241	Molecular Biophysics I	30 Sept
Rontani Massimo	#103	Magnetism and Spin related phenomena II	29 Sept
Rosi Gabriele	#529	Metrology	2 Oct
Rossetti Giulia	#003	Computational Biophysics I	28 Sept
Rossi Giulia	#072	Computational Biophysics II	29 Sept
Rossini Davide	#316	Correlated electrons and cold atoms	1 Oct
Rovigatti Lorenzo	#380	Soft Matter I	1 Oct
Ruffino Francesco	#562	Advanced materials for energy applications III	2 Oct
Ruffo Stefano	#079	Interdisciplinary statistical physics.	29 Sept
Ruggeri Rosa	#545	Electronical and optical properties of low dimensional systems III	2 Oct
Ruggerone Paolo	#002	Computational Biophysics I	28 Sept
Ruggieri Sonia	#609	Complexity in the brain	2 Oct
Ruoso Giuseppe	#129	Quantum Fluctuations and Casimir Forces	29 Sept
Sabbioni Cristina	#499	Environmental Physics and Pollution	2 Oct
Sada Cinzia	#232	Optofluidics	29 Sept
Saitta A. Marco	#405	Molecular liquids in equilibrium and non-equilibrium regimes	1 Oct

Sala Vittorio	#476	Advanced Microscopy Techniques	2 Oct
Salasnich Luca	#317	Correlated electrons and cold atoms	1 Oct
Salluzzi Marco	#098	Magnetism and Spin related phenomena II	29 Sept
Sanchez Pedro A.	#272	Magnetism and Spin related Phenomena III	30 Sept
Sangaletti Luigi	#441	Nanomaterials and Nanotechnology: carbon nanotubes	1 Oct
Sant Marco	#178	Noncovalent interactions: advances in Computer Simulations	29 Sept
Santoro Mario	#630	Synchrotron radiation and material science II	2 Oct
Saracco Fabio	#497	Econophysics	2 Oct
Sartori Paolo	#249	Statistical Mechanics of Active Matter	30 Sept
Sassi Alberto	#568	Molecular Biophysics II	2 Oct
Satriano Cristina	#351	Gas Sensors and Biosensors for Health and Wealth	1 Oct
Savasta Salvatore	#057	Nanophotonics I	28 Sept
Savio Letizia	#088	From nanoparticles to nanostructured surfaces	29 Sept
Sberveglieri Veronica	#350	Gas Sensors and Biosensors for Health and Wealth	1 Oct
Scaini Denis	#440	Nanomaterials and Nanotechnology: carbon nanotubes	1 Oct
Scala Antonio	#168	Diffusion and reaction in complex systems	29 Sept
Scala Matteo	#337	Quantum Optics and Coherent Manipulation	1 Oct
Scalas Enrico	#491	Econophysics	2 Oct
Scamarcio Gaetano	#043	Optical feedback and metamaterials in mid-IR and THz	28 Sept
Scarangella Adriana	#365	Advanced Optical Materials I	1 Oct
Schillaci Francesco	#265	Plasma Physics IV	30 Sept
SCHIRO GIORGIO	#240	Molecular Biophysics I	30 Sept
Sciarrino Fabio	#427	Quantum thermodynamics and quantum technologies 1	1 Oct
Sciortino Alice	#442	Nanomaterials and Nanotechnology: carbon nanotubes	1 Oct
Sciortino Francesco	#461	Soft Matter II	1 Oct
Sciortino Luisa	#557	Synchrotron radiation and material science I	2 Oct
Sciortino Luisa	#619	Advanced optical characterization techniques	2 Oct
Scopece Daniele	#087	From nanoparticles to nanostructured surfaces	29 Sept
Scordino Agata	#478	Advanced Microscopy Techniques	2 Oct
Scuderi Viviana	#117	Oxide Films and Interfaces	29 Sept
Scuto Andrea	#211	Sustainable Nanotechnologies III	29 Sept
Scuto Andrea	#389	Advanced materials for energy applications I	1 Oct
Selva Anna	#509	Dosimetry	2 Oct
Serafini Luca	#553	Synchrotron radiation and material science I	2 Oct
Sessoli Roberta	#031	Magnetism and spin related phenomena I	28 Sept



Sharma Parikshit	#354	Gas Sensors and Biosensors for Health and Wealth	1 Oct
Sheverdyeva Polina	#190	Magnetism and Spin related phenomena IV	29 Sept
Shwartz Sharon	#418	New physics with ultrashort light and x-ray pulses II	1 Oct
Siciliano Pietro	#356	Gas Sensors and Biosensors for Health and Wealth	1 Oct
Silva Fernández Blanca	#328	New physics with ultrashort light and x-ray pulses I	1 Oct
Sirleto Luigi	#479	Advanced Microscopy Techniques	2 Oct
Solinas Paolo	#430	Quantum thermodynamics and quantum technologies 1	1 Oct
Sorba Lucia	#459	Electronic and optical properties of low dimensional systems II	1 Oct
Spagnolo Bernardo	#481	Out of Equilibrium Statistical Mechanics I	2 Oct
Spagnolo Salvatore	#130	Quantum Fluctuations and Casimir Forces	29 Sept
Spagnolo Vincenzo	#154	THz and Quantum Cascade Lasers	29 Sept
Spelta Alessandro	#495	Econophysics	2 Oct
Spilla Samuele	#517	Quantum thermodynamics and quantum technologies 2	2 Oct
Spirito Davide	#225	2D emerging materials II	29 Sept
Strano Vincenzina	#213	Sustainable Nanotechnologies III	29 Sept
Strelkov Vasily	#063	Laser-Matter Interaction: from Atoms to Nano-Particles	28 Sept
Suma Antonio	#395	Biophysical Models II	1 Oct
Suzuki Satoru	#227	2D emerging materials II	29 Sept
Svergun Dmitri	#236	Molecular Biophysics I	30 Sept
Taccogna Francesco	#183	Plasma Physics III	29 Sept
Tajfirouze Edris	#094	Plasma Physics II	29 Sept
Tamburello Giancarlo	#591	Physical Processes in Volcanic Eruptions	2 Oct
Tanjia Fatema	#263	Plasma Physics IV	30 Sept
Tardocchi Marco	#025	Plasma Physics I	28 Sept
Terrasi Antonio	#217	Photovoltaic materials and devices	29 Sept
Tiana Guido	#305	Biophysical Models I	1 Oct
Tiribocchi Adriano	#251	Statistical Mechanics of Active Matter	30 Sept
Tocchio Luca Fausto	#315	Correlated electrons and cold atoms	1 Oct
Toci Guido	#623	Advanced optical characterization techniques	2 Oct
Tomadin Andrea	#222	2D emerging materials II	29 Sept
Tornari Vivi	#322	Imaging and non-destructive analysis	1 Oct
Torrisi Felice	#139	2D emerging materials I	29 Sept
Totani Roberta	#138	2D emerging materials I	29 Sept
Traina Paolo	#523	Diamond-based substrates and Memristors for Brain sensing	2 Oct
Trillo Stefano	#538	Fiber and Miniaturized Optical Sensors	2 Oct

Troia Benedetto #147	Nanophotonics II	29 Sept
Trovato Antonio	#157 Computational Biophysics III	29 Sept
Tubiana Luca #394	Biophysical Models II	1 Oct
Urbinati Giulia #304	Photonic and plasmonic materials and devices	30 Sept
Urru Andrea #615	Nanomaterials and Nanotechnology: Graphene	2 Oct
Urso Riccardo Giovanni #050	Sustainable Nanotechnologies I	28 Sept
Uversky Vladimir N.	#566 Molecular Biophysics II	2 Oct
Vaccaro Lavinia	#451 Advanced Optical Materials II	1 Oct
Valenti Luca #209	Sustainable Nanotechnologies III	29 Sept
Valentinis Davide Filippo	#040 Cuprates and Mechanisms for Superconductivity	28 Sept
Vanderzande Carlo	#247 Statistical Mechanics of Active Matter	30 Sept
Vandin Giulio #161	Computational Biophysics III	29 Sept
Vanossi Andrea #084	From nanoparticles to nanostructured surfaces	29 Sept
Varagnolo Silvia	#233 Optofluidics	29 Sept
Veranda Marco #264	Plasma Physics IV	30 Sept
Verdini Alberto #432	Organic on Substrates III	1 Oct
Verna Adriano #329	New physics with ultrashort light and x-ray pulses I	1 Oct
Vilasi Silvia #567	Molecular Biophysics II	2 Oct
Virgili Tersilla #423	New physics with ultrashort light and x-ray pulses II	1 Oct
Vitali Lucia #457	Electronic and optical properties of low dimensional systems II	1 Oct
Viti Leonardo #058	Nanophotonics I	28 Sept
Vitiello Miriam Serena #149	THz and Quantum Cascade Lasers	29 Sept
Viviani Massimo	#125 Sustainable Nanotechnologies II	29 Sept
Wlodarski Wojtek	#348 Gas Sensors and Biosensors for Health and Wealth	1 Oct
Wuite Gijs #475	Advanced Microscopy Techniques	2 Oct
Yeomans Julia #244	Statistical Mechanics of Active Matter	30 Sept
Zamuner Stefano	#308 Biophysical Models I	1 Oct
Zeng Hao #258	Light Manipulation	30 Sept
Zhou Xingjiang #106	Iron Based Superconductors	29 Sept
Zivieri Roberto #101	Magnetism and Spin related phenomena II	29 Sept
Zizzari Alessandra	#235 Optofluidics	29 Sept
Zoli Marco #465	Soft Matter II	1 Oct
Zontone Federico	#629 Synchrotron radiation and material science II	2 Oct
Zuena Martina #324	Imaging and non-destructive analysis	1 Oct
Zyss Joseph #291	Non Linear Optics	30 Sept