#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_2-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 $–NH_2$ 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_2 up to Pd_9 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.

[1] M. Terrones, J. M. Romo-Herrera, E. Cruz-Silva, F. López-Urías, E. Muñoz-Sandoval, J. J. Velázquez-Salazar, H. Terrones, Y. Bando, D. Golberg, *Mater. Today*, 2007, 10, 30.
[2] M. Renzhi , B. Yoshio , Z. Hongwei, S. Tadao, Xu Cailu, Wu Dehai, J. Am. Chem. Soc., 2002, 124 , 7672
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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_{30} 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^{1} 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 determing step requiring 95.7 kJ mol^{1}.

[1] R.D. Cortright, R.R. Davda, J.A. Dumesic Nature, 2002, 418, 964-967
[2] I.L. Godina, A.V. Kirilin, A.V. Tokarev, D. Yu Murzin, ACS Catal., 2015, 5, 2989-3005

#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 Plexigas tank of 50 cm x 30.3 cm x 7.5 cm equipped with a removable banner 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