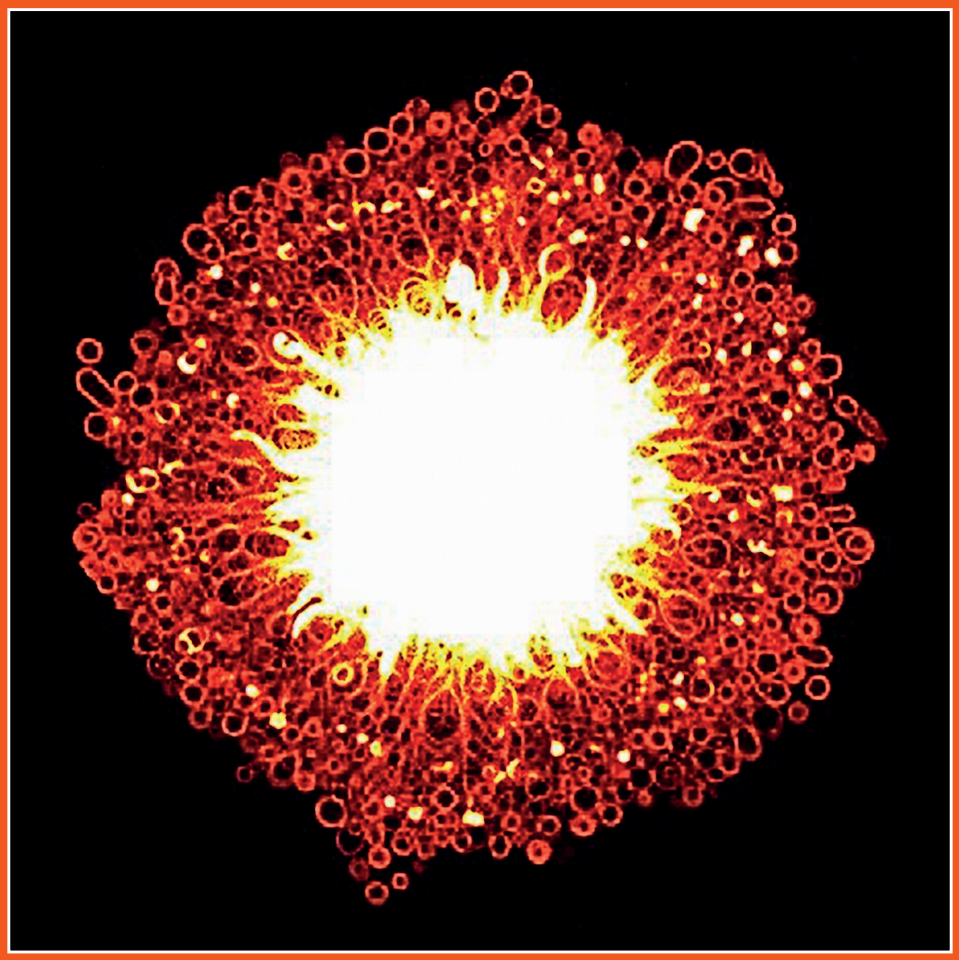
Programme and Abstracts

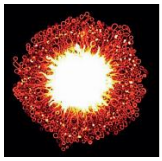


The Physics of Soft and Biological Matter

14–16 April 2014
Homerton College, Cambridge, UK

Organised by IOP Biological Physics Group, IOP Liquids and Complex Fluids Group, IOP Molecular Physics Group and IOP Polymer Physics Group

IOP Institute of Physics



The Physics of Soft and Biological Matter

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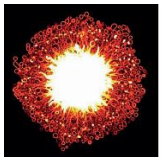

The Physics of Soft and Biological Matter

Welcome

Welcome to the conference on The Physics of Soft and Biological Matter! We are looking forward to inspiring presentations and stimulating discussions throughout the three days.

Our programme consists of 50 contributed lectures organised into eight parallel sessions, along with more than 100 posters in two sessions with multiple viewings. Highlighting the programme are six invited lectures from world-leading scientists on topics spanning the diverse subject of soft matter and biological physics.

Our programme is organised around several core topics:

- Biological Systems
- Colloids and Nanoparticles
- Confined Fluids and Interfacial Phenomena
- Liquids, Glasses and Liquid Crystals
- Polymers, Polyelectrolytes and Biomolecules
- Surfactants, Foams and Emulsions

Additionally, there are three cross-cutting themes that link together these topics:

- Optical Methods and Imaging
- Rheology and Non-equilibrium Phenomena
- Self-Assembly, Biomimetics, and Pattern Formation

We expect that the conference will facilitate a cross-fertilisation of ideas between researchers in different aspects of soft matter and biological physics. By bringing us all together at a single meeting, the complementarity of concepts and phenomena will be more apparent.

Our programme committee is comprised of members representing four different Groups of the UK's Institute of Physics: Biological Physics Group; Liquids and Complex Fluids Group; Molecular Physics Group; and Polymer Physics Group. The meeting has been organised in response from the desire of our Group members to have a forum to exchange ideas and to develop collaborations, rather than looking inward towards our own specialist interests. This conference follows on from two previous conferences with the same name, which were hosted by the Universities of Nottingham and Warwick.

We are fortunate to have financial support from four exhibitors: Biolin Scientific, HORIBA Scientific, IOP Publishing and LOT Quantum Design. Please look for their exhibits in the Boulind Suite and learn about their latest range of products. If you have any questions about any aspect of the arrangements, please contact us or one of the Institute of Physics Conference staff members (Joanne Hemstock or Dawn Stewart), who are on-site throughout the three days. We welcome your feedback. Enjoy your stay in Cambridge!

The Programme Committee

Michael Allen (Warwick); Giuseppe Battaglia (UCL); Martin Buzza (Hull); Pietro Cicuta (Cambridge); Neil Hunt (Strathclyde); Joseph Keddie (Surrey)

Programme

Monday 14 April

11:30	Registration *Porter's Lodge, Mary Allen Building*	
12:00	Lunch *Great Hall*	
13:20	**Welcome address** J L Keddie, University of Surrey, UK	
Chair: M P Allen, University of Warwick, UK		
13:30 – 14:15	**(Invited) Hydrodynamics and phase behaviour of active suspensions** S Fielding, Durham University, UK *Auditorium*	
	Rheology of Active and Biological Matter *Auditorium* **Chair:** M P Allen, University of Warwick, UK	**Confined Fluids and Interfacial Phenomena** *John Hammond Lecture Theatre* **Chair**: M Buzza, University of Hull, UK
14:20	**Rheology and shear-induced diffusion of dense red blood cell suspensions** T Krueger, University of Edinburgh, UK	**Capillary force on a micrometric sphere trapped at a fluid interface exhibiting arbitrary curvature gradients** M Nobili, CNRS / Université Montpellier 2, France
14:35	**Motility fractionation of bacteria by centrifugation** C Maggi, Università di Roma "Sapienza", Italy	**Capillary fluctuations, interface potential and the film height dependent surface tension of adsorbed liquid films** L G MacDowell, Universidad Complutense de Madrid, Spain
14:50	**Bacterial delivery of colloids over anisotropic barriers** N Koumakis, Università di Roma "Sapienza", Italy	**Relaxation of surface tension in the liquid-solid interfaces of Lennard-Jones liquids** A V Lukyanov, University of Reading, UK
15:05	**Active matter at high density** S Henkes, University of Aberdeen, UK	**Off-equilibrium surface tension in colloidal suspensions** D Truzzolillo, CNRS / Université Montpellier 2, France
15:20	**Viscoelastic response of actin networks at intermediate distances** A Sonn-Segev, Tel Aviv University, Israel	**Structure of photo-responsive semifluorinated alkanes at the water-air interface** A Theodoratou, FORTH / University of Crete, Greece
15:35	**Poster session A, exhibition and refreshments** *Boulind Suite*	
	Biological Systems *Auditorium* **Chair:** G Battaglia, University College London, UK	**Colloids and Nanoparticles** *John Hammond Lecture Theatre* **Chair:** M P Allen, University of Warwick, UK
16:15	**Similar emergent states in swarming animals and thermophoretic colloids** M S Turner, University of Warwick, UK	**Near-wall dynamics of spherical colloids: Translational and rotational diffusion** M Lisicki, University of Warsaw, Poland
16:30	**Emergent run-and-tumble in a simple model of Chlamydomonas** R Bennett, University of Oxford, UK	**Asphaltene deposition in microfluidic capillary flow experiments and particulate computer simulation** C M Seifried, Imperial College London, UK
16:45	**Microswimmer motilty in rigid and elastic confinement** R Ledesma-Aguilar, Northumbria University, UK	**Colloidal musical chairs - String- and loop-like cooperative motion in locally perturbed 2D colloidal crystals** J Sprakel, Wageningen University, The Netherlands
17:00	**Clathrin aggregation by rotational brownian dynamics** I M Ilie, University of Twente, The Netherlands	**How do platinum janus particles swim?** A Brown, University of Edinburgh, UK
17:15	**Self-organisation of swimming bacteria in confined geometries** H Wioland, University of Cambridge, UK	**Hydrodynamic synchronisation of simple rotors** S Box, University of Bristol, UK
17:30	**Poster session A, exhibition and refreshments** *Boulind Suite*	
18:30	Break	
19:30	Dinner *Great Hall*	

Tuesday 15 April

08:00	Breakfast (residential guests only) *Great Hall*	
Chair: J L Keddie, University of Surrey, UK		
09:00 - 09:45	**(Invited) Capillary-driven flow in thin polymer films** K Dalnoki-Veress, McMaster University, Canada *Auditorium*	
	Polymers, Polyelectrolytes and Biomolecules *Auditorium* **Chair:** J L Keddie, University of Surrey, UK	**Self-Assembly, Biomimetics and Pattern Formation** *John Hammond Lecture Theatre* **Chair:** G Battaglia, University College London, UK
09:50	**Unwinding dynamics of polymers: a model for single biomolecules?** J-C Walter, University Montpellier 2, France	**Enzyme-driven chemotactic synthetic vesicles** D Cecchin, University College London, UK
10:05	**Threading dynamics of ring polymers in a gel** D Michieletto, University of Warwick, UK	**Encapsulating hydrogenase active site analogues in peptide-based supramolecular hydrogels: a photochemical study** P W J M Frederix, University of Strathclyde, UK
10:20	**New method to predict the surface tension of complex synthetic and biological polyelectrolyte/surfactant mixtures** R A Campbell, Institut Laue-Langevin, France	**Motility-induced phase separation in an active dumbbell fluid** G Gonnella, Università di Bari, Italy
10:35	**Kinetic control over out-of-equilibrium self-assembled hydrogels** V D Nguyen, Wageningen University, The Netherlands	**Atom-scale computer-aided design of organic-inorganic interfaces** D Thompson, University of Limerick, Ireland
10:50	**Poster session A, exhibition and refreshments** *Boulind Suite*	
	Biological Systems *Auditorium* **Chair:** N Hunt, University of Strathclyde, UK	**Rheology and Non-equilibrium Phenomena** *John Hammond Lecture Theatre* **Chair:** P Cicuta, University of Cambridge, UK
11:30	**The role of intrinsically disordered proteins under conditions of abiotic stress** F Yuen, University of Cambridge, UK	**Length-scale dependent aging and plasticity of a colloidal polycrystal under cyclic shear** E Tamborini, Université Lyon 1, France
11:45	**Traffic jams on the microtubule network** D Miedema, University of Amsterdam, The Netherlands	**Particle response during the yielding transition of colloidal glasses** D V Denisov, Van der Waals-Zeeman Institute, The Netherlands
12:00	**Multiscale self-assembly of fibrin governs its polymerization kinetics, fiber and network structure, as well as nonlinear rheological properties** N A Kurniawan, FOM Institute AMOLF, The Netherlands	**Molecular dynamics simulations of flow in nanopores** D A Ross, Imperial College London, UK
12:15	**Nanoscale ligand spacing influences receptor triggering in immunological synapses** I E Dunlop, Imperial College London, UK	**Microfluidic-SANS: in situ molecular insight into non-equilibrium phenomena in complex fluids** C G Lopez, Imperial College London, UK
12:30	**Exploring the molecular bases of cytoskeleton-cell membrane interactions, by live imaging approach** L Chierico, University College London, UK	**Interfacial rheology of model particles at liquid interfaces** J H J Thijssen, University of Edinburgh, UK
12:45	Lunch *Great* Hall	
Chair: G Battaglia, University College London, UK		
14:00 - 14:45	**(Invited) Scaling laws of polymer membranes: from synthetics to nuclear envelopes and mechanotransduction** D E Discher, University of Pennsylvania, USA *Auditorium*	
	Self-Assembly, Biomimetics and Pattern Formation *Auditorium* **Chair:** G Battaglia, University College London, UK	**Confined Fluids and Interfacial Phenomena** *John Hammond Lecture Theatre* **Chair:** M P Allen, University of Warwick, UK
14:50	**Orientational texture of lipid membrane domains** A Cohen Simonsen, University of Southern Denmark, Denmark	**Crystal-liquid interfacial free energy via thermodynamic integration** R Benjamin, Heinrich-Heine Universitaet, Germany

Tuesday 15 April continued

15:05	**Phase separation within hybrid polymer/lipid vesicles used as biomimetic membranes** J F Le Meins, Bordeaux University, France	**Circularly confined quasi-hard-discs: the role of boundary adaptivity** I Williams, University of Bristol, UK
15:20	**Photo cross-linked and pH sensitive polymersomes - nanoreactor and membrane studies** J Gaitzsch, University College London, UK	**Displacement mechanisms in micro-models from micro-fluidic experiments and pore scale lattice Boltzmann simulations** E S Boek, Imperial College London, UK
15:35	**Poster session B, exhibition and refreshments** *Boulind Suite*	
Chair: M Buzza, University of Hull, UK		
16:15 - 17:00	**(Invited) Directed assembly in soft matter** K J Stebe, University of Pennsylvania, USA *Auditorium*	
	Surfactants, Foams and Vesicles *Auditorium* **Chair:** M Buzza, University of Hull, UK	**Optical Methods and Imaging** *John Hammond Lecture Theatre* **Chair:** N Hunt, University of Strathclyde, UK
17:05	**Unveiling the bifurcation diagram of pattern formation in surfactant monolayer transfer** M H Koepf, École Normale Supérieure, France	**Exploring soft matter with X-ray scanning micro- and nano-diffraction techniques** E Di Cola, European Synchrotron Radiation Facility (ESRF), France
17:20	**Extreme deformation of giant unilamellar vesicles in a complex shear flow** A Pommella, Imperial College London, UK	**Single cell monitoring of redox potential using Surface-enhanced Raman Spectroscopy** K Fisher, University of Edinburgh, UK
17:35	**Foams stabilized by mixtures of nanoparticles and oppositely charged surfactants: Relationship between bubble shrinkage and foam coarsening** A Maestro, University of Cambridge, UK	**Optical Coherence Tomography Velocimetry of complex fluids** A V Malm, University of Manchester, UK
17:50	**Poster session B, exhibition and refreshments** *Boulind Suite*	
18:30	Break	
19:30	Conference dinner *Great Hall*	

Wednesday 16 April

08:00	Breakfast (residential guests only) *Great Hall*	
Chair: M Buzza, University of Hull, UK		
09:00 - 09:45	**(Invited) Self-assembly of patchy colloids** D J Pine, New York University, USA *Auditorium*	
	Colloids and Nanoparticles *Auditorium* **Chair:** M Buzza, University of Hull, UK	**Self-Assembly** *John Hammond Lecture Theatre* **Chair:** G Battaglia, University College London, UK
09:50	**Phase diagrams for magnetic nanofilaments** J J Cerdà, Universidad de las Islas Baleares, Spain	**Epitaxy and polymorph selection in heterogeneous crystal nucleation** J P Mithen, University of Surrey, UK
10:05	**Colloidal aggregation and dynamics in anisotropic fluids** O Mondain-Monval, University of Bordeaux, France	**Simulation of polymer network formation: Phase behavior of aggregating chains** H Mortazavi, Eindhoven University of Technology, The
10:20	**The effects of polydispersity and metastability on colloidal crystallization** R M L Evans, University of Leeds, UK	**Dynamic renormalisation group theory reveals sequential mechanism of oligomer generation in protein aggregation** T C T Michaels, University of Cambridge, UK

Wednesday 16 April continued

10:35	**Poster session B and refreshments** *Boulind Suite*	
Chair: J L Keddie, University of Surrey, UK		
11:15 - 12:00	**(Invited) Single molecule studies of protein aggregation** D Klenerman, University of Cambridge, UK *Auditorium*	
	Colloids and Nanoparticles *Auditorium* **Chair:** J L Keddie, University of Surrey, UK	**Liquid Crystals** *John Hammond Lecture Theatre* **Chair:** M P Allen, University of Warwick, UK
12:05	**Ligand-mediated nanoparticle interactions at fluid-fluid interfaces** V Garbin, Imperial College London, UK	**On phase behaviour and dynamical signatures of charged platelet suspensions** S Jabbari-Farouji, University of Joseph-Fourier, France
12:20	**Studying complex nanoparticle adsorption at liquid interfaces** A Nelson, ETH Zürich, Switzerland	**Knotted defects in nematic liquid crystals** T Machon, University of Warwick, UK
12:35	**Design of a fluorinated magneto-responsive material with tuneable ultrasound scattering properties** K Zimny, University of Bordeaux, France	**Double twist liquid crystal model of collagen structure** A Brown, Dalhousie University, Canada
12:50	Lunch *Great Hall*	

Poster Session A (afternoon of 14 April and morning of 15 April)

Biological systems

P.01 Mechanotransduction of deformable nano-structured elastic membrane surfaces on proliferation of osteoblast cells
G K Toworfe, Flowers School of Technology and Management, Germany / University of Pennsylvania, USA

P.02 Streaming potential in human dentin
Z Feng, Xiamen University, China

P.03 Structure and evolution of high-density protein systems
J Ioannou, University of Cambridge, UK

P.04 Dynamics of filopodium-like protrusion and endothelial cellular motility on 1-D extracellular matrix fibrils
Y Y S Huang, University of Cambridge, UK

P.05 Modelling of the Nuclear Pore Complex
D Osmanovic, University College London, UK

P.06 Effect of solvent on the self-assembly of Dialanine and Diphenylalanine Peptides
A N Rissanou, University of Crete, Greece / IACM FORTH, Greece

P.07 Double-belt a novel structure of membrane pore
R Vacha, Masaryk University, Czech Republic

P.08 Induced guidance of NIH 3T3 fibroblasts on Polydimethylsiloxane (PDMS) ridge-groove substrates: a time-lapse live-cell study
C-K Huang, University of Cambridge, UK

P.09 Influence of Ibupropfen on the structure of phospholipid layers
S Jaksch, Forschungszentrum Jülich GmbH, Germany

P.10 Study of cellular differentiation of embryonic carcinoma stem cells by AFM nanocytomechanics and Raman spectroscopy
E Canetta, St Mary's University College, UK

P.11 New insight into the structure and function of Hfq carboxyl terminus
V Arluison, University Paris Diderot, France/CEA, France

P.12 Single cell measurements of intracellular signaling, and motility, in activated macrophages
E Cammarota, University of Cambridge, UK

Colloids and nanoparticles

P.13 Restricted diffusion of small probe particles in a laponite dispersion
S Kaloun, SAEED Ecole Supérieure de Technologie Essaouira, Université Cadi Ayyad, Morocco

P.14 Dynamic properties of concentrated microgel suspensions and protein solutions
J Riest, Forschungszentrum Jülich GmbH, Germany

P.15 Detachment energies of spheroidal particles from liquid-liquid interfaces
G Davies, University College London, UK

P.16 Bicontinuous emulsions stabilized by nanoparticles
M Reeves, University of Edinburgh, UK

P.17 Controlling ink properties to achieve a 'flatter' film profile for applications in P-OLED displays
A D Eales, University of Cambridge, UK

P.18 Influence of magnetic field on the orientation of anisotropic magnetic particles at liquid interfaces
B J Newton, University of Hull, UK

Confined fluids and interfacial phenomena

P.19 Effective interaction between a colloid and a soft interface near criticality
A D Law, Max-Planck-Institut für Intelligente Systeme, Germany

P.20 Adsorption energies of poly(ethylene oxide)-based surfactants and nanoparticles on an air-water surface
A Nelson, ETH Zurich, Switzerland

P.21 Analysis of an axisymmetric two-phase flow model for particle transport at fluid interfaces
L Botto, Queen Mary University of London, UK

Optical methods and imaging

P.22 Dual-mode microviscosity measurements in lipid monolayer and bilayer systems with a molecular rotor
A Vysniauskas, Imperial College London, UK

P.23 Imaging dynamic patterns in lipid membranes using molecular rotors
M R Dent, Imperial College London, UK

P.24 A Label-Free Microfluidic Assay to quantitatively study antibiotic diffusion through lipid membranes
J Cama, University of Cambridge, UK

P.25 Simple continuum descriptions of macromolecule complexes for imaging techniques
C Prior, Durham University, UK

Polymers, polyelectrolytes and biomolecules

P.26 Modifications of the study of dielectric properties of a polycarbonate plastic (Makrofol KG) induced by Si^{7+} heavy ion irradiation
M Mujahid, University of Tabuk, Saudi Arabia

P.27 Pickering emulsion polymerized core-shell structured smart composite particles and their suspension rheology under electric and magnetic fields
H J Choi, Inha University, Korea

P.28 Passive and active microrheology of a polymer melt studied by molecular dynamics simulation
A Kuhnhold, Martin-Luther-Universitaet Halle-Wittenberg, Germany

P.29 Microscobic probing of melting and gelation processes in well-defined biopolymer network
H E Cingil, Wageningen University, The Netherlands

P.30 Tunable reversible hydrogels from metal-coordinated polymers
M Bohdan, Wageningen University, The Netherlands

P.31 Two-fluid model for ions distribution on a charged surface: A Monte Carlo study and modified Poisson-Boltzmann theory
C-H Cheng, National Changhua University of Education, Taiwan

P.32 The role of confinement and interaction range on polarisation and alignment of stiff chains and networks
K K Müller-Nedebock, Stellenbosch University, South Africa

P.33 Inert-tail effect on the thermodynamics of DNA hybridisation
L Di Michele, University of Cambridge, UK

P.34 Large-area patterning of the tackiness of a colloidal nanocomposite adhesive by sintering of nanoparticles under IR radiation
J L Keddie, University of Surrey, UK

P.35 Lubrication by polymersomes under nanoconfinement
J E Bartenstein, University of Bristol, UK

Rheology and non-equilibrium phenomena

P.36 Spatio-temporal dynamics of collective flow across a bacterial carpet
Y-T Hsiao, National Central University Taiwan, China

P.37 Surface roughening due to patchy particles in (1+1) dimensions - A computational study
M J Kartha, University of Pune, India

P.38 Lipid bilayer membranes under shear flow from molecular simulations
A Botan, Université Lyon 1, France

P.39 The tube axis and entanglements in polymer melts
A Likhtman, University of Reading, UK

Self-assembly, biomimetics and pattern formation

P.40 From wound healing to artificial muscles: Modelling bio- and biomimetic materials with polar and nematic order parameters
M H Koepf, École Normale Supérieure, France

P.41 Dynamical Landau theory for the assembly and disassembly kinetics of supramolecular polymers
N Tiwari, Eindhoven University of Technology, The Netherlands

P.42 Engineering DNA-linked janus liposome clusters towards applications in drug delivery
T Wild, University of Leeds, UK

P.43 All-optical manipulation of photonic membranes
B Kirkpatrick, University of St. Andrews, UK

P.44 Self-assembly of nanoparticles on fluid membranes
A Saric, University of Cambridge, UK

P.45 Inherent variability in the kinetics of autocatalytic protein self-assembly
J Szavits-Nossan, University of Edinburgh, UK

P.46 Understanding the self-assembly and structure of interfacial films formed from the bacterial hydrophobin BslA
R J Morris, University of Edinburgh, UK

P.47 Self-assembly of naphthalene-dipeptides to form hydrogel films at the air-water interface
T Li, University of Edinburgh, UK

Surfactants, foams and emulsions

P.48 Dynamic wetting of hydrophobic polymers by aqueous surfactant and superspreader solutions
X Wang, Technical University Darmstadt, Germany

P.49 Atomistic description of the solubilisation of testosterone propionate in a sodium dodecyl sulfate micelle
D Allen, King's College London, UK

Poster Session B (afternoon of 15 April and morning of 16 April)

Biological systems

P.01 Force localization in contracting cell layers
C Dunlop, University of Surrey, UK

P.02 Orientational order and motility in active droplets
D Khoromskaia, University of Warwick, UK

P.03 Fluctuating finite element analysis: Modelling biomacromolecules with continuum mechanics
D Read, University of Leeds, UK

P.04 Dynamics of oblate and prolate capsules in shear flow
Y Sui, Queen Mary University of London, UK

P.05 Mechanical properties of keratin fibres in complex environments
R Notman, University of Warwick, UK

P.06 Ion channel gating by electrokinetic interactions
D J Bonthuis, University of Oxford, UK

P.07 Variable temperature single molecule force spectroscopy of an extremophilic protein
K Tych, University of Leeds, UK

P.08 Modelling the transport of nanoparticles across the blood-brain barrier
G Fullstone, University College London, UK

P.09 Folding of cellular monolayers
S Hoehn, University of Cambridge, UK

P.10 Active polar fluid flow in deformable droplets
C A Whitfield, University of Sheffield, UK

P.11 Is it possible the hydrodynamic synchronization of colloidal rotors describing rigid trajectories? - an experimental proof
A Maestro, University of Cambridge, UK

P.12 Short-time dynamics E. coli chromosomal loci reveal a dependence on coordinate and indicate the presence of a sporadic but ubiquitous super-diffusive motion
A Javer Godinez, University of Cambridge, UK

Colloids and nanoparticles

P.13 Design concepts for nanostructured colloidal composites
J L Keddie, University of Surrey, UK

P.14 Nucleation of hard colloidal cubes
C Karner, University of Vienna, Austria

P.15 The reciprocal theorem for two objects
D Papavassiliou, University of Warwick, UK

P.16 PNIPAM microgels: A novel insight into their adsorption at fluid interfaces
A Maestro, University of Twente, The Netherlands / University of Cambridge, UK

P.17 Unusual order in squeezed spheres
W G Ellenbroek, Eindhoven University of Technology, The Netherlands

P.18 Deposition of colloidal asphaltene in capillary flow from computer simulation and homogeneous deposition models
E S Boek, Imperial College London, UK

Confined fluids and interfacial phenomena

P.19 Predicting anomalous fluid densities in carbon nanotubes
G J Wang, MIT, USA

P.20 Direct effects of non-equilibrium aggregates on Pdadmac/SDS layers at the air/water interface
I Varga, Eötvös Loránd University, Hungary

P.21 A Landau-Squire nanojet
N Laohakunakorn, University of Cambridge, UK

P.22 Hindered diffusion coefficients of spherical particles confined by microchannels
K Misiunas, University of Cambridge, UK

Liquid crystals/Liquids and glasses

P.23 Crystallization mechanism in melts of short n-alkane chains
M Anwar, Université du Luxembourg, Luxembourg

P.24 Effect of temperature on orientational ordering in a modified Gay-Berne fluid
R C Singh, Vidya College of Engineering, India

P.25 Electron transitions in Cr^{2+} in the aqueous solutions of $MgSO_{3.6}H_2O$:Cr
I Ismailov, Shumen University, Bulgaria

Polymers, polyelectrolytes and biomolecules

P.26 Cross-sectional imaging of organic solar cells: Understanding efficiency and lifetime issues
T Glen, University of Cambridge, UK

P.27 Computational studies on the effect of stereotacticity of poly(N-isopropylacrylamide) in aqueous solution
V Botan, RWTH University, Germany

P.28 MD and COSMO-RS contact statistics for poly(N-isopropylacrylamide) in solvents
V Botan, RWTH University, Germany

P.29 Transition path sampling with core-modification aimless shooting for a homopolymer chain
C Leitold, University of Vienna, Austria

P.30 Self-assembly of degalatosylated xyloglucan from tamarind seeds
D Bulone, Biophysics Institute, National Research Council, Italy

P.31 Key factors regulating the mass delivery of macromolecules to model cell membranes: gravity and electrostatics
R A Campbell, Institut Laue-Langevin, France

P.32 Hydration dynamics of proteins in solutions studied in 220–325 GHz band
O Sushko, Queen Mary University of London, UK

P.33 Nanostructuring thin polymer films with 2 and 3-beam single pulse laser interference lithography
I Martín-Fabiani, Instituto de Estructura de la Materia (IEM-CSIC), Spain

Rheology and non-equilibrium phenomena

P.34 Active nematic dynamics in a viscoelastic background
E Hemingway, Durham University, UK

P.35 Simulation of the linear and non-linear rheology of viscoelastic polymer solutions
B W Fitzgerald, University of Twente, the Netherlands

P.36 Plastic deformation mechanisms in glassy and semi-crystalline polymers
S Jabbari-Farouji, University of Joseph-Fourier-Grenoble, France

P.37 Dynamics and structure: a study of gelation in a non-aqueous colloidal system
F R Bartholomew, University of Cambridge, UK

Self-assembly, biomimetics and pattern formation

P.38 Lattice model of nucleation via partially disordered precursor
Y Lifanov, University of Warwick, UK

P.39 Fibrous scaffolds for neural tissue engineering in the auditory system
K Ngamkham, University College London, UK

P.40 Hierarchical morphogenesis of a hybrid peptide/protein system
K E Inostroza, Queen Mary University of London, UK; Nanotechnology Platform, Parc Científic de Barcelona, Spain

P.41 Synthetic DNA viruses for targeting breast cancer cells
L Guan, University College London, UK

P.42 Design of patchy polymersomes with topological surface patterns at the nanoscale
L Messager, University College London, UK

P.43 Fabrication of "intelligent nanosurfaces" for controlled cell- substrate interaction
P Mokarian-Tabari, University College Cork and Tyndall National Institute, Ireland; Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Ireland

P.44 Artificial DNA membrane nanopores
K Göpfrich, University of Cambridge, UK

P.45 Out of equilibrium pattern formation in lipid membranes
L Parolini, University of Cambridge, UK

Surfactants, foams and emulsions

P.46 Surfactants and aqueous solubility enhancement of drugs: importance of the hydrophilic "head group"
Y Saaka, King's College London, UK

P.47 Pickering emulsion by arresting phase separation using anisotropic particles
S V Daware, Indian Institute of Technology, India

P.48 Immiscible lipids control the morphology of patchy emulsions
L-L Pontani, New York University, USA

FORTHCOMING INSTITUTE CONFERENCES
MAY 2014 – JULY 2016

2014

19–24 May
9th International Workshop on Neutrino-Nucleus Interactions in the Few-GeV Region: NuInt14
Selsdon Park Hotel, Surrey, UK
Organised by the IOP High Energy Particle Physics Group

9–11 July
3rd Superconductivity Summer School
University of Oxford, Oxford, UK
Organised by the IOP Superconductivity Group

14–15 July
Colloidal Quantum Dots and Nanocrystals
Chancellors Hotel and Conference Centre, Manchester, UK
Organised by the IOP Quantum Electronics and Photonics Group

14–16 July
Dielectrophoresis 2014
Institute of Physics, London, UK
Organised by the IOP Electrostatics Group

15–17 July
"Innovative Instrumentation for EURISOL" 5th EURISOL Topical Meeting 2014
University of York, York, UK
Organised by the IOP Nuclear Physics Group

21–25 July
ICSOS'11: 11th International Conference on the Structure of Surfaces
University of Warwick, Coventry, UK
Organised by the IOP Thin Films and Surfaces Group

26–28 August
IPTA 2014: Inverse Problems from Theory to Application
At-Bristol, Bristol, UK
Organised by IOP Publishing

1–4 September
Photon14
Imperial College London, London, UK
Organised by the IOP Computational Physics, Instrument Science and Technology, Optical, Quantum Electronics and Photonics and Quantum Information, Quantum Optics and Quantum Control Groups

3–5 September
Physics meets Biology
University of Oxford, Oxford, UK
Organised by the IOP Biological Physics Group

4–5 September
International Conference on the History of Physics
University of Cambridge, Cambridge, UK
Organised by the IOP History of Physics Group

15–19 September
Quantum, Atomic, Molecular and Plasma Physics (QuAMP) Summer School
Durham/Newcastle University, UK
Organised by the IOP Atomic and Molecular Interactions, Molecular Physics, Plasma Physics, Quantum Electronics, and Photonics and Quantum Optics, Quantum Information and Quantum Control Groups

16–18 December
Topical Research Meeting on Hybrid Quantum Systems
National College for Teaching and Leadership, Nottingham, UK
Organised by the IOP Quantum Optics, Quantum Information and Quantum Control Group

2015

30 March – 2 April
Interdisciplinary Surface Science Conference (ISSC-20)
University of Birmingham, Edgbaston, UK
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Oral Abstracts

Monday 14 April

(invited) Hydrodynamics and phase behaviour of active suspensions

S Fielding

Durham University, UK

We simulate a suspension of active squirming disks over the full range of volume fractions from dilute to close packed, with full hydrodynamics in two spatial dimensions. Doing so, we show that "motility induced phase separation" (MIPS), recently proposed to arise generically in active matter, is strongly suppressed by hydrodynamic interactions. We give an argument for why this should be the case, and support it with counterpart simulations of active Brownian disks in a parameter regime more closely suited to hydrodynamic suspensions than in previous studies. Time permitting, another project concerning the rheology of active suspensions will also be outlined, discussing results obtained within continuum models of active nematohydrodynamics.

Rheology of Active and Biological Matter

Rheology and shear-induced diffusion of dense red blood cell suspensions

M Gross[1], T Krueger[2] and F Varnik[1,3]

[1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany, [2]School of Engineering, University of Edinburgh, UK, [3]Max-Planck Institut für Eisenforschung, Germany

Suspensions of soft particles are ubiquitous. One of the most popular and biologically important examples is blood which is a moderately dense (volume fraction 45%) suspension of red blood cells (RBCs) and other, less abundant constituents. While the rheology and shear-induced diffusion of hard sphere suspensions is relatively well understood, this is less so for suspensions of soft particles. Due to their deformability and aspherical shape, additional time scales and degrees of freedom are present and a theoretical description is more complicated.

In this talk we will present recent progress in the field, supported by combined lattice-Boltzmann-immersed boundary-finite-element computer simulations (Figure 1). Motivated by the dynamical properties of RBCs under confinement, it is possible to construct an effective theoretical model and to predict the viscosity of blood over a remarkably large parameter range, spanning several orders of magnitude in shear rate as well as volume fractions between 10 and 90%. The dependence on shear rate and volume fraction of the shear-induced diffusivity of RBCs can be largely understood by considering the solvent flow in the gaps between the particles. We recover canonical behaviour in the Newtonian regime and a characteristic power-law scaling at high volume fractions and shear rates. Our results are helpful to understand rheological effects in dense soft particle suspensions and to predict suspension properties based on their microscopic features and external control parameters.

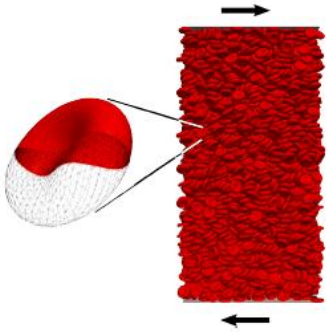

Figure 1: Dense RBC suspension under shear (right) and numerical mesh of a RBC (left).

[1] T. Krueger, M. Gross, D. Raabe, F. Varnik. Crossover from tumbling to tank-treading-like motion in dense simulated suspensions of red blood cells. Soft Matter 9, 9008-9015, 2013

[2] M. Gross, T. Krueger, F. Varnik. Rheology of dense suspensions of elastic capsules: yield stress, jamming and confinement effects. Submitted, http://arxiv.org/abs/1401.2914

[3] M. Gross, T. Krueger, F. Varnik. Fluctuations and diffusion in athermal suspensions of deformable particles. Submitted.

Motility fractionation of bacteria by centrifugation

C Maggi[1], A Lepore[2,3], J Solari[1], A Rizzo[1] and R Di Leonardo[1]

[1]Dipartimento di Fisica, Università di Roma "Sapienza", Italy, [2]Dipartimento di Matematica e Fisica, Universita' degli Studi di Roma Tre, Italy, [3]CNR-IPCF UOS Roma, Italy

Flagellar motility plays a fundamental biological role in prokaryotic and eukaryotic unicellular organisms. Modulating flagellar activity in response to a variety of chemical and physical stimuli, single-celled micro-organisms can effectively search for optimal environmental conditions. Flagellar motility also plays an important role in medicine, being a major contributing factor to pathogenicity and colonization in bacteria like *Vibrio cholerae*. More recently, the possibility of exploiting swimming micro-organisms as actuators for microstructures has extended the interest for flagellar motility to the physical domain of micro-engineering applications[1,2]. Recognizing the primary role of motility has led to the development of new tools that are capable of a precise and quick characterization of the dynamical properties of cells. Image correlation techniques, as dynamic image correlation spectroscopy (ICS) and differential dynamic microscopy (DDM), are promising tool offering a high-throughput method for characterizing the motility of microorganisms[3].

However, in conjunction to physical tools for motility quantification, it is also desirable to develop physical techniques for sorting colonies, that usually display a high motility variation, into spatially separated fractions characterized by a motility gradient. Fractionation by centrifugation is a widely used technique in biology and chemistry. It relies on the strong sensitivity of sedimentation speed on particle size and composition and therefore allows to separate components according to size, mass or density. As a result a stationary state is eventually reached where, each solute is distributed according to the Boltzmann law: $\rho\ (z)\ \propto \exp[-v_d z/D]$, with $v_d = \mu \Delta m a$ is the drift speed induced by a uniform centrifugal acceleration a on a particle having a buoyant mass Δm, mobility μ and a diffusion coefficient $D\ = \mu k_B T$. Although bacteria will display some variations in the buoyancy mass, we do not expect it to be strongly correlated to their motility. On the other hand swimming bacteria do not rely on thermal agitation for motion, but have their own source of propelling power that makes them a strongly out of equilibrium system. It has been found that in many respects, they can be thought of as "hot colloids", with an effective diffusivity that strongly depends on motility and that is typically hundreds of times larger than the Brownian diffusivity of non-motile cells[4].

In this talk we experimentally demonstrate[5] that a sample of motile *E. coli* bacteria, displaying a broad spectrum of swimming speeds, behaves like a mixture of "hot" colloids having a corresponding broad spectrum of effective temperatures and therefore sedimentation lengths (see Fig. 1). As a consequence, after centrifugation, non-motile bacteria will accumulate to the bottom of the cell while higher regions are populated with bacteria having an increasing motility/temperature. We used ICS to perform space-resolved motility measurements of bacteria observed over a field of view spanning 1 mm. Space dependent motility distribution were retrieved for centrifugal fields in the range ~ 4-12 g and accounted for with a simple theoretical model of active diffusion.

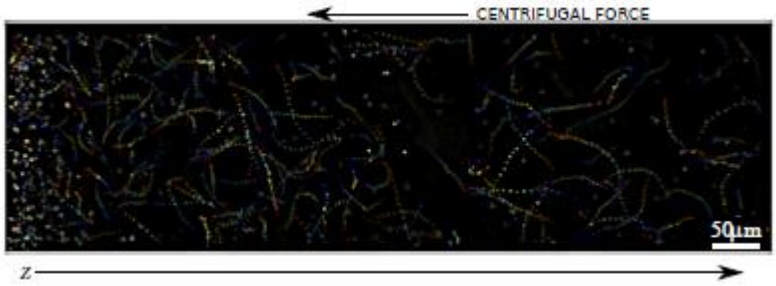

FIG. 1: Traces of swimming bacteria after centrifugation obtained from digital-videomicroscopy. Slow bacteria are found sedimented at the bottom of the sample (left-hand side) while faster ones populate the high-z region of the sample. Traces are obtained as a superposition of frames that have been colored progressively from red to blue as time increases.

[1] R. Di Leonardo al., PNAS, 107, 9541, (2010)
[2] L. Angelani, C. Maggi, et al. PRL, 107, 138302, (2011)
[3] V. A. Martinez, R. Besseling, O. A. Croze, et al. Biophys. Journal, 103 1637 (2012)
[4] M. E. Cates., Rep. Prog. Phys. 75 042601 (2012)
[5] C. Maggi et al., Soft Matter, 9 10885 (2013)

Bacterial delivery of colloids over anisotropic barriers

N Koumakis[1], A Lepore[1,2,3], C Maggi[3] and R Di Leonardo[1,3]

[1]CNR-IPCF UOS Roma, Italy, [2]Dipartimento di Fisica, Università di Roma Tre, Italy, [3]Dipartimento di Fisica, Università di Roma "Sapienza", Italy

Exploiting motile micro-organisms for the transport of colloidal cargoes is a fascinating strategy to extract work from self-propelled entities. Generally, delivery on target sites requires external control fields to steer propellers and trigger cargo release. This need of a constant feedback prevents the design of compact devices where biopropellers could perform their tasks autonomously. Here we experimentally show that properly designed three-dimensional micro-structures can define accumulation areas where bacteria spontaneously and efficiently spatially organize colloidal beads[1]. The mechanism does not require modification of colloidal cargoes nor any external control fields, rather the process is stochastic in nature and results from the rectifying action of an asymmetric energy landscape over the fluctuating forces arising from collisions with swimming bacteria. As a result, the concentration of colloids over target areas can be strongly increased or depleted according to the topography of the underlying structures. Besides the significance to technological applications, our experiments pose some important questions regarding the structure of stationary probability distributions in non-equilibrium systems. To address some of these issues, simulations employing varying classes of time-correlated noise have been employed, showing that the details of applied noises may significantly alter the steady state probability distributions over asymmetric barriers.

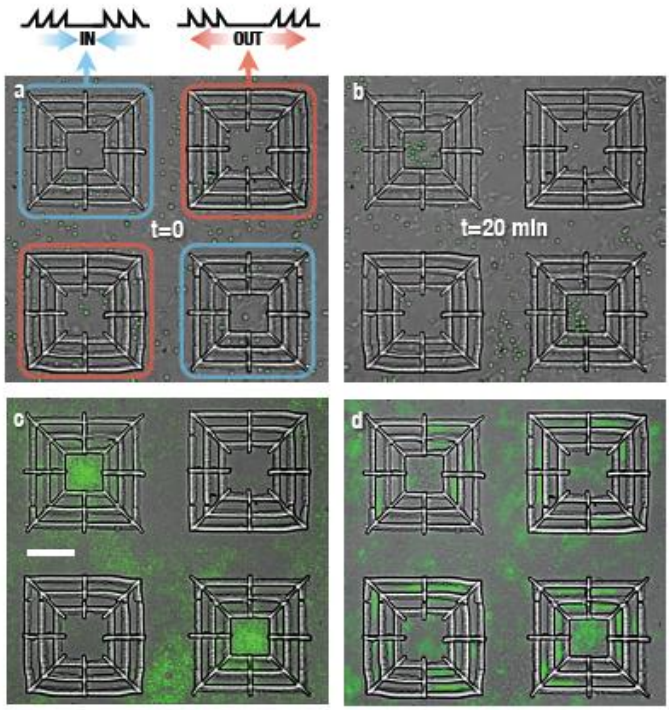

FIG. 1: Observation of particle concentration and depletion by bacteria. Single experiment snapshots of particles and bacteria at the initial state $t = 0$ where particles are randomly distributed (panel a) and for $t = 20\ min$, where particle distributions have been strongly affected by bacterial transport over asymmetric barriers (panel b). Particle distributions averaged over a steady state are shown in panel c for particles in the bacterial bath between $t1 = 15\ min$ and $t2 = 20\ min$ ($\Delta t = 5\ min$) and in panel d for particles in an experiment without bacteria, undergoing simple Brownian motion for $\Delta t = 10 min$. In the absence of bacteria, the colloidal particles remain trapped within the structures compartments. The scale bar in panel c is 20 μm in length.

[1] N. Koumakis, C. Maggi, A. Lepore and R. Di Leonardo, “Targeted delivery of colloids by swimming bacteria" Nat. Comm.4, 2588 (2013) doi: 10.1038/ncomms3588

Active matter at high density

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[1]ICSMB, Department of Physics, University of Aberdeen, UK, [2]Department of Physics, Brandeis University, USA, [3]Department of Physics and Syracuse Biomaterials Institute, Syracuse University, USA

Active matter is a rapidly growing field that has potential applications to biological systems from the organism scale to the sub-cellular level. A key outstanding question relevant especially to biological tissues remains the behaviour of active particle systems at high density. In an effort to map the fundamental properties of dense active materials, we perform a numerical study of a dense collection of self-propelled particles with soft repulsive interactions in two dimensions. Incorporating self propulsion as a force and alignment as a torque into fully overdamped equations, our model is an appropriate template for active colloids and similar systems.

In a first system with alignment, we observe an active jammed phase at high density and low self-propulsion speed (Figure 1, left). The dynamics of this phase is controlled by the low-frequency modes of the underlying jammed packing, in a reverse fluctuation cascade from the microscale to global oscillations.

The non-aligning system was recently shown to exhibit active phase separation in two dimensions in the absence of any attractive interaction or breaking of the orientational symmetry. We construct a phase diagram in terms of

activity and packing fraction and identify three distinct regimes: a homogeneous liquid with anomalous cluster size distribution, a phase-separated state both at high and at low density, and a frozen glassy phase with fluctuations resembling dynamical heterogeneities and shear flow.

We develop scaling arguments for the melting transition and for the boundaries separating the liquid and the cluster phase in both the low and high density regions.

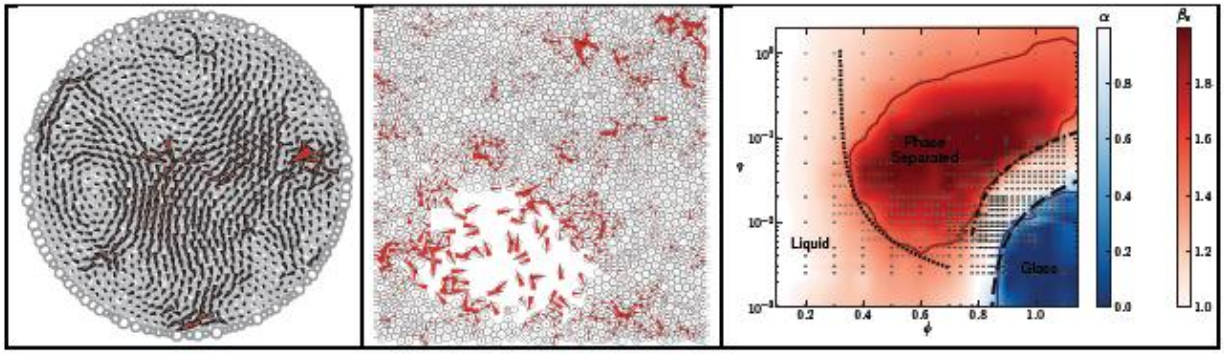

Figure 1: Simulated dense active systems. Left: Confined aligning system in the active jammed phase, red arrows represent particle velocity. Middle: High density clustering phase for the non-aligning system. Right: Phase diagram in the packing fraction and self propulsion axes for the non-aligning system, showing the locations of the glassy phase (blue) and the clustering phase (deep red).

Viscoelastic response of actin networks at intermediate distances

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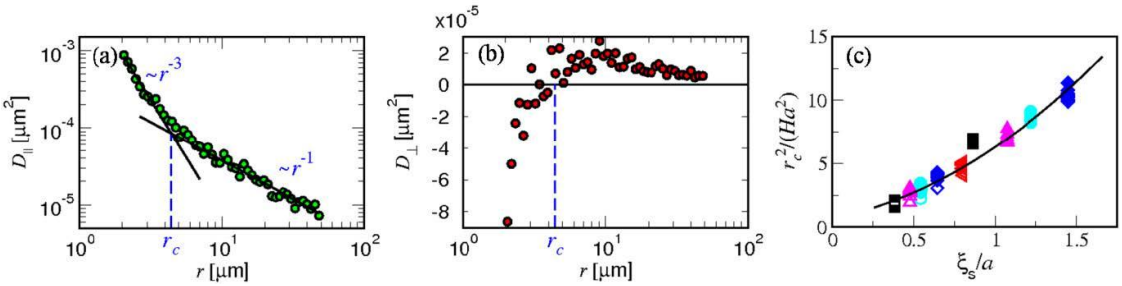
The viscoelastic response of actin networks is length- and time-scale dependent, encoding information on intrinsic dynamic correlations and mesoscopic structure. Over sufficiently large distances the network responds as a continuous medium, characterized by frequency dependent viscoelastic moduli. But how large should the distance be for this asymptotic bulk limit to hold?

We report the observation of a large-distance intermediate response in an experimental system of entangled F-actin gels. The tools of 1-point and 2-point microrheology were used to characterize the local and distance-dependent responses of the actin networks, respectively.

The 2-point response at intermediate distances, arising from the effect of mass displacement rather than momentum diffusion, is enhanced by the much softer local microenvironment of the tracers compared to the bulk properties of the gel. Consequently, the cross-over to the bulk behavior is pushed to surprisingly large distances, much larger than the mesh size, ξ_s, of the actin gel. Results from several networks with different mesh sizes will be presented, emphasizing this inherent property of complex fluids and its relation to ξ_s. This intermediate response has implications for the micro-scale dynamics of cells.



(a) Longitudinal and (b) transverse displacement correlations as a function of particle separation at lag time $\tau = 0.014\,\mathrm{sec}\; for\; \xi_s = 0.44\;\mu m$ and tracer's particle radius $a = 0.55\;\mu m$. The cross-over distance r_c (blue dashed line) is defined at the intersection of the fitted dominant (r^{-1}) and subdominant (r^{-3}) power-law decays of $D_{\parallel}$. (c) Cross-over distance for different α and ξ_s , colors and symbols correspond to different ξ_s. Open (filled) symbols correspond to $= 0.55\;(0.245)\;\mu m$. All experimental results fall on a master curve once r_c^2 is normalized and present as a function of ξ_s/a . The solid line is a fit to the theoretical prediction.

[1] A. Sonn-Segev, A. Bernheim-Groswasser, H. Diamant and Y.Roichman, accepted to Phys. Rev. Lett. (arXiv:1307.4278)

Confined Fluids and Interfacial Phenomena

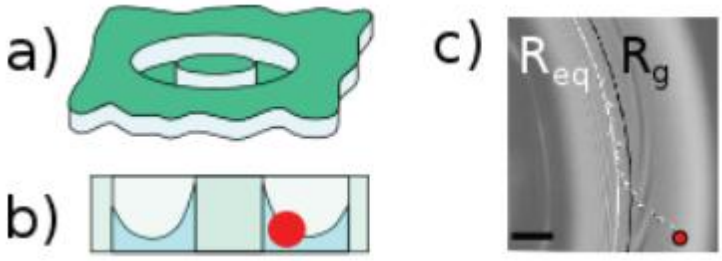
Capillary force on a micrometric sphere trapped at a fluid interface exhibiting arbitrary curvature gradients

C Blanc[1,2], D Fedorenko[1,2], M Gross[1,2], M In[1,2], M Abkarian[1,2], M A Gharbi[1,2], J-B Fournier[3], P Galatola[3] and M Nobili[1,2]

[1]Université Montpellier 2, France, [2]CNRS, Laboratoire Charles Coulomb, France, [3]Université Paris Diderot, France

Strong normal restoring forces due to the surface tension are sufficient to confine solid objects at fluid interfaces. In many studies, the interface is planar and spatially uniform, merely providing a 2D confinement on particles. When curved, interfaces might play a more active role, imposing a lateral force on the particles. A spectacular demonstration of this force is the meniscus-climbing technique of the beetle larva [1]. In the presence of a curved interface, the mechanical equilibrium conditions at the triple line larva/water/air impose an extra surface deflection and thus a lateral force on the larva. This force is also sufficient to drive micron-long cylinders self-assembly on a water/air curved interface [2]. Despite these interesting studies a full comparison between experiment and theory is still lacking.

In this Letter [3], we combine theory and experiment to address the capillary force acting on a spherical colloid placed on a curved fluid interface. We develop a new theoretical model able to predict this force in the general case of interfaces with arbitrary curvature. Using a built-in interferometric method coupled with particle tracking, we measured the femto-Newton forces which control the equilibrium position of microspheres. We found a good agreement with our theoretical predictions. Our findings open the way to the control of the force and the assembly of micrometric size particles by the design of the interface morphology.



a) top view and b) side view of the experimental cuvette. Also drawn in b) the designed mineral oil/air interface having a gradient of gaussian curvature with a trapped bead (in red). c) Superposed images of bead trajectory in bright field and of interface morphology by Mirau interferometry. A bead partially embedded in oil overpasses its gravity potential minimum R_g (black arc), climbs the slope and finally reaches an equilibrium radius R_{eq} (white arc) with $R_{eq} < R_g$. Bar indicate 5 µm.

[1] D. L. Hu and J. W. M. Bush, *Nature* (London) 437, 733 (2005)
[2] M. Cavallaro, L. Botto, E. P. Lewandowski, M. Wang, and K. J. Stebe, *Proc. Natl. Acad. Sci.* U.S.A. 108,20 923, (2011)
[3] Christophe Blanc, Denys Fedorenko, Michel Gross, Martin In, Manouk Abkarian, Mohamed Gharbi, Jean-Baptiste Fournier, Paolo Galatola and Maurizio Nobili, *Physical Review Letter*, 111, 058302 (2013)

Capillary fluctuations, interface potential and the film height dependent surface tension of adsorbed liquid films

L G MacDowell[1], J Benet[1], N A Katcho[2] and J M G Palanco[3]

[1]Department Química Física, Faculty Química, Universidad Complutense de Madrid, Spain, [2]LITEN, CEA-Grenoble, France, [3]Escuela de Ingeniería Aeronáutica Universidad Politécnica de Madrid, Spain

The Capillary Wave Hamiltonian (CWH) lays at the heart of most theoretical accounts of surface phenomena, including, renormalization group analysis of wetting transitions, the study of droplet profiles, or the prediction of line tensions.

The virtue of this model is that it allows to predict the behavior of complex film morphologies solely from the properties of a flat film. Namely, the *interface potential*, $g(\ell)$, defined as the free energy of a flat film of height ℓ, and the liquid–vapor surface tension, γ_{lv}. This is achieved by defining a film profile, $\ell(x)$, that describes the film height on each point of the underlying plane. The CWH is constructed as a functional of $\ell(x)$, which assumes a free energy $g\ell(x)$, locally, but includes extra contributions due to bending of the interface via the liquid–vapor surface tension:

$$H\left[\ell\left(x\right)\right] = \int \left\{g\left(\ell\left(x\right)\right) + \gamma_{lv}\sqrt{1 + \left[\nabla\,\ell\left(x\right)\right]^2}\right\} dx \qquad (1)$$

where $H[\ell]$ is the free energy of the complex film profile. Application of this result to the study of thermal capillary waves on an adsorbed flat film provides the following expectation for the spectrum of film height fluctuations:

$$\frac{k_B\,T}{A < \left|\ell_q\right|^2 >} = g^{"}_{cws} + \gamma_{cws}\,q^2 + O(q^4) \qquad (2)$$

where ℓ_q are the Fourier modes of the film height fluctuations, while $g^{"}_{cws}$ and γ_{cws}, are coefficients of the polynomial expansion in powers of the wave vector **q**. According to the classical model, the coefficient $g^{"}_{cws} = d^2\,g(\ell)/d\ell^2$, while $\gamma_{cws} = \gamma_{lv}$.

In this paper we perform computer simulations of the capillary wave spectrum of an adsorbed film and show for the first time that [1,2]:

- The coefficient $g^{"}_{cws}$ precisely follows the second derivative of $g(\ell)$as obtained independently from thermodynamic integration.
- The second order coefficient, γ_{cws} is asymptotically equal to γ_{lv}, but picks–up an additional film thick dependence, which we show accurately follows $\gamma\,(\ell) = \gamma_{lv} + \xi^2 g^{"}\,(\ell)$, where ξ is the bulk correlation length.

Our theoretical approach shows for the first time that the film height dependence $\gamma\,(\ell)$ follows from a hitherto unnoticed capillary wave broadening mechanism beyond mere interfacial displacements. Accordingly, the interfacial roughness, of order $\langle\delta\ell^2\rangle$ in the classical theory, takes an additional contribution $\langle(\nabla\ell)^2\rangle$ of order square gradient. This conclusion is shown to agree with expectations from Renormalization Group Theory.

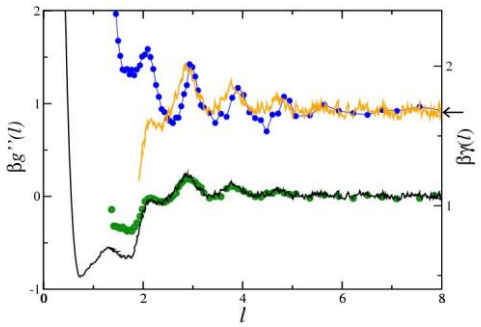


FIG. 1. Interface potentials (left axis) and surface tension (right axis) of adsorbed liquid films. Green symbols are results for $g''(\ell)$ as obtained from the CWS. Black lines are results from the interface potential as determined by thermodynamic integration. Blue symbols are results for $\gamma(\ell)$ as obtained from the CWS, while the orange lines correspond to our theoretical estimate $\gamma(\ell) = \gamma_{lv} + \xi^2 g''(\ell)$. The arrow points to the value of γ_{lv} obtained independently from the virial.

[1] L. G. MacDowell, J. Benet and N. A. Katcho, Phys. Rev. Lett. 111, 047802 (2013)
[2] L. G. MacDowell, J. Benet and N. A. Katcho, J. M. G. Palanco, Adv. Colloid Interface Sci. DOI:10.1016/j.cis.2013.11.003 (2013)

Relaxation of surface tension in the liquid-solid interfaces of Lennard-Jones liquids

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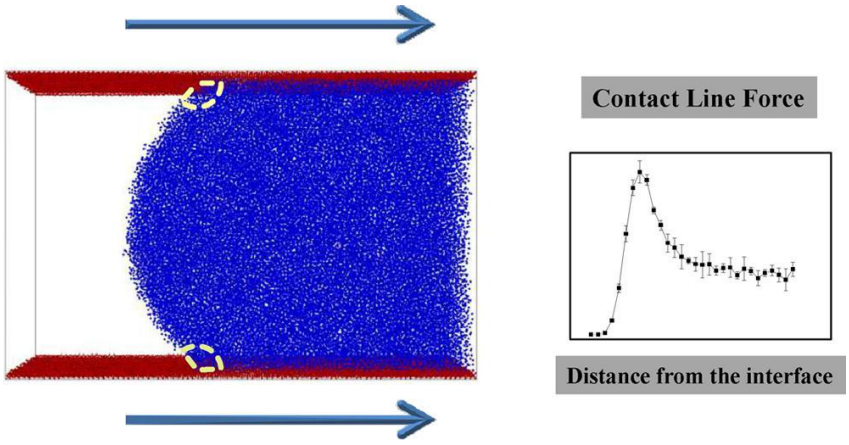
We have established the surface tension relaxation time in the liquid-solid interfaces of Lennard-Jones simple and complex liquids by means of direct measurements in molecular dynamics (MD) simulations. The main result is that the relaxation time is found to be independent of the molecular structures (the chain length) and viscosity of the liquids (at 70-fold change) used in our study and lies in such a range that in slow hydrodynamic motion the interfaces are expected to be at equilibrium. This has been also verified in the direct MD experiments on dynamic wetting, where the dynamic contact angle was observed. The implications of our results for the modelling of dynamic wetting processes and interpretation of dynamic contact angle data are discussed. In particular, we compare with the existing models and directly demonstrate the mechanism of dynamic contact angle generation at nanoscale.



Off-equilibrium surface tension in colloidal suspensions

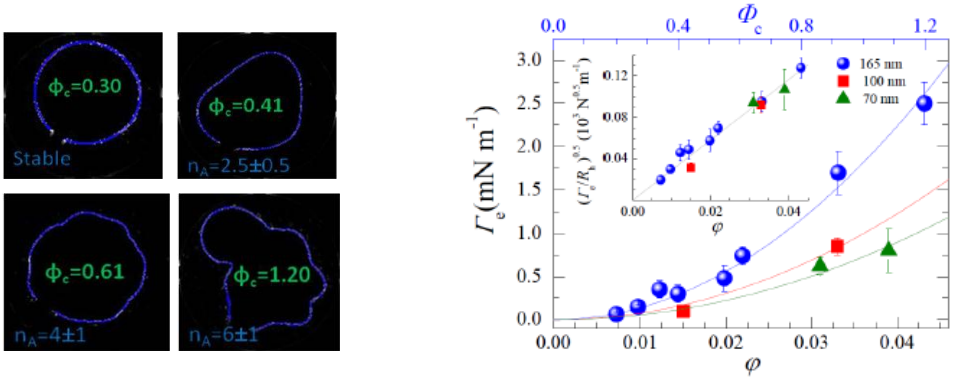
D Truzzolillo[1,2], S Mora[1,2], C Dupas[1,2] and L Cipelletti[1,2]

[1]Université Montpellier 2, France, [2]CNRS, France

Surface tension between immiscible fluids is a well-understood and well-characterized phenomenon. By contrast, much less is known about the effective, off-equilibrium surface tension that arises when a (transient) interface is created between *miscible* fluids. This effective surface tension plays a key role in many phenomena, from jetting and drop formation and coalescence to precipitation and deposition, as it was already recognized more than 100 years ago by Korteweg [1], who first hypothesized that effective surface tensional stresses must be at work between two miscible fluids at contact. However, experimental investigations in this field remain scarce and the theoretical predictions by Korteweg have not quantitatively tested so far, to the best of our knowledge. We present a thorough experimental investigation of the Saffman-Taylor instability arising when a simple fluid (the solvent of a colloidal suspension) is pushed through a miscible, more viscous one (the colloidal suspension itself). We show [2] that the

resulting interface pattern can be accounted for by the non-linear rheological properties of the suspension and an effective surface tension. By measuring the effective surface tension for suspensions at a variety of particle volume fractions, we successfully test Korteweg's theory.

We moreover find that the effective surface tension *increases* with the size of the colloidal particles, a surprising result at odd with the typical behavior in atomic or colloidal systems, where the surface tension usually *decreases* as the squared particle size [3]. We rationalize this finding by showing that for our particles, microgel spheres composed of cross-linked polymers, the surface tension is dominated by the entropic contribution associated with the internal degrees of freedom of the polymers



Left panel: Observed patterns in a Hele-Shaw radial experiment right after the onset of fingering instability at a fixed injection rate and different effective microgel volume fraction Φ_c as indicated in the panels. The average number of observed fingers n_A is also shown [2]. Right panel: Effective interfacial tension Γe between the microgel suspensions and their solvent, as a function of colloid (resp., polymer) volume fraction (top, resp. bottom, axis). The lines are quadratic fits to the data for microgels with various hydrodynamic radii, as shown by the legend.

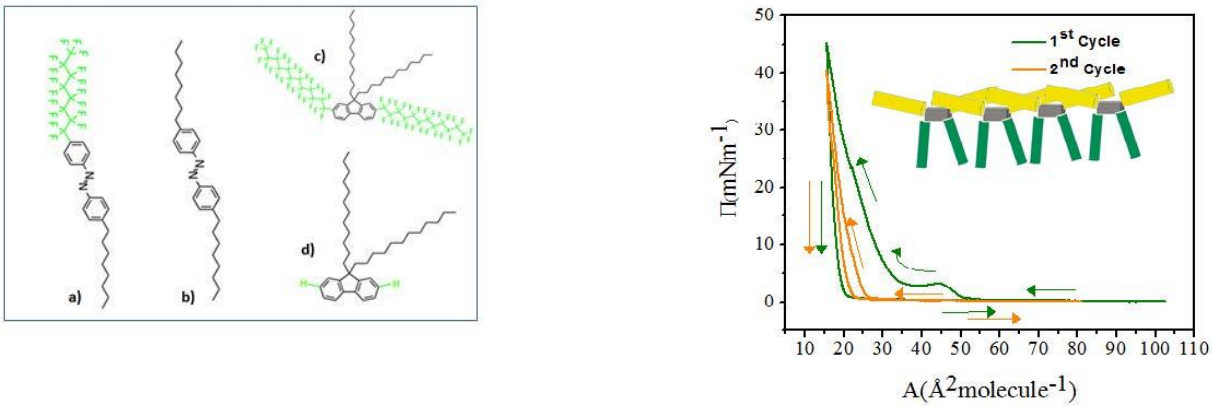
[1] D. Korteweg, Arch. Neerlandaises Sci. Exactes Naturelles, 6, 1 (1901)
[2] D.Truzzolillo, S. Mora, C. Dupas, L. Cipelletti, http://arxiv.org/abs/1312.4427 (Submitted)
[3] P.-G. de Gennes, F. Brochard-Wyart, and D. Queré, Capillarity and Wetting Phenomena: Drops, Bubbles, Pearls, Waves (Springer-Verlag, Berlin, 2004)

Structure of photo-responsive semifluorinated alkanes at the water-air interface

A Theodoratou[1,2], U Jonas[3], B Loppinet[1], T Geue[4] and D Vlassopoulos[1,2]

[1]FORTH, Institute of Electronic Structure & Laser, Greece, [2]University of Crete, Greece, [3]University of Siegen, Germany, [4]Laboratory for Neutron Scattering, Paul Scherrer Institut, Switzerland

The structural properties of semifluorinated alkanes (SFA) at the water-air interface have received attention over the last years because of their ability to form stable Langmuir monolayers at the air-water despite the hydrophobicity of both constituents. This allows tailoring film properties for specific applications. In the present study we investigate the effects of molecular architecture and external stimuli on the interfacial properties of a novel series of architecturally complex semifluorinated alkanes. They include a T-shaped fluorene derivative with four side chains (FL(HH12)9(FF12)2,7) and an analogous without fluorinated side chains (FL(HH12)9(HH2)2,7) (figure 1). A systematic investigation of structure formation in response to light stimulus has been performed for semifluorinated azobenzene derivatives (F8-azobenzene-H8 and H8-azobenzene-H8) at the water-air interface and after transfer to the silicon wafers.



Left panel: Chemical structure of SFAs a) F8-azobenzene-H8, b) H8-azobenzene-H8, c) FL(HH12)9(FF12)2,7 and d) FL(HH12)9(HH2)2,7 Right panel: Surface pressure isotherm of FL(HH12)9(FF12)2,7 and the proposed molecular packing from neutron reflectivity analysis at the water-air interface

We apply the methodology developed recently to study the two-dimensional packing behavior of semifluorinated alkanes with varying architecture e.g., with a central C-C bond in the molecule, *F*12*H*12 [1] [2]. We study the hierarchical self-assembly by means of neutron reflectivity, pressure isotherms and compression-expansion cycles using a Langmuir trough. We find that the UV irradiation influence dramatically the packing behavior of the azobenzene molecules leading from vertically oriented structures to mixed configurations with any signature of phase transition. We show that the fluorinated T-shaped molecules form layers undergoing a phase transition (Π=3mN/m-see figure) and irreversible compression-expansion deformation. On the other hand, for hydrogenated molecules with the same structure, a reversible layer deformation without any phase transition is detected. Packing models of both systems are proposed thanks to the analysis of neutron reflectivity spectra.

[1] de Viguerie L., Keller R., Jonas J., Berger R., Clark C., Klein C., Geue T., Muller K., Butt H.J., Vlassopoulos D. , Langmuir 27 (2011) 8776

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Biological Systems

Similar emergent states in swarming animals and thermophoretic colloids

D J G Pearce, A Tamsett, G Rowlands and M S Turner

University of Warwick, UK

Bird flocks, insect swarms and fish shoals resemble fluids made up of many individuals where the controlling interactions are social rather than physical in character [1]. Some progress has been made reverse-engineering candidates for these interactions that are local in space, either in a metric-based [2] or topological sense [3,4]. A question that has been largely overlooked is whether the interactions should be expected to be local at all. We discuss the evidence for them having a non-local character and, furthermore, that there is a natural choice for this that is consistent with the cognitive limitations of a bird's vision. This leads us to propose a non-local *hybrid-projection* model. This has the physically satisfying feature that it involves an unusually small number of control parameters, when compared with other swarming models. We study the global character of the flocks that emerge from this model and their various phenotypes. Most significantly, an emergent state arises in which the probability that a typical bird can see out (sky) in any direction divided by the probability that its view is blocked by other bird(s) is O(1). We refer to this as *marginally opaque*, see Fig 1. We present experimental data on bird flocks that

confirm this prediction and discuss how these models may naturally be associated with evolutionary fitness, as well as being physiologically plausible.

Finally we report on recent work on systems of thermophoretic colloids that are heated by an external light source, extending on [5]. We show that these systems can undergo first order transitions from compact to disperse states as the light intensity is varied. Intriguingly, we find that the same state of marginal opacity emerges: no compact state with a density below marginal opacity is stable. This reveals an unexpected similarity between social and thermodynamic swarms.

Figure 1: The centre panel is an image of a real flock of Starlings. It is *marginally opaque*. The left and right panels show the same image artificially doctored so as to resemble states that would have a very low (<<1) or a very high (≈1) opacity, respectively.

[1] I. Giardina, *Collective behaviour in animal groups: theoretical models and empirical studies*. HFSP Journal 2, 205 (2008)

[2] T. Vicsek., A. Czirók, E. Ben-Jacob, I. Cohen, O. Shochet, *Novel type of phase transition in a system of self-driven particles*. Phys. Rev. Lett. 75, 1226 (1995)

[3] A. Cavagna et al., *Scale-free correlations in starling flocks.* PNAS 107, 11865 (2010).

[4] M. Ballerini et al., *Empirical investigation of starling flocks: a benchmark study in collective animal behaviour.* Anim. Behav. 76, 201 (2008)

[5] J. A. Cohen and R. Golestanian, *Emergent cometlike swarming of optically driven thermally active colloids*, arXiv:1309.3318 and accepted for publication in Phys. Rev. Lett. (2014)

Emergent run-and-tumble in a simple model of Chlamydomonas

R Bennett and R Golestanian

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The green alga *Chlamydomonas* has two flagella which beat in synchrony with a breaststroke like motion. I consider a simple hydrodynamic model consisting of three spheres, shown in figure1, from which we see interesting features in the synchronization behaviour. The flagella need to have a phase dependent beat pattern during forward motion in order to synchronize. Rapid synchronization occurs from the hydrodynamic friction due to cell rotation, while hydrodynamic interactions are only a second order effect. Some beat patterns lead to synchronization and others do not [1]; this enables the model to produce run-and-tumble behaviour when we add intrinsic noise [2], in agreement with experimental observations [3]. Figure 2 shows an example of a run-and-tumble trajectory produced by the model. Some beat patterns may or may not lead to synchronization, depending on the initial conditions. The model is simple, yet provides a wide range of different types of behaviour, giving the possibility of using the model to study other features in the motion of *Chlamydomonas*.

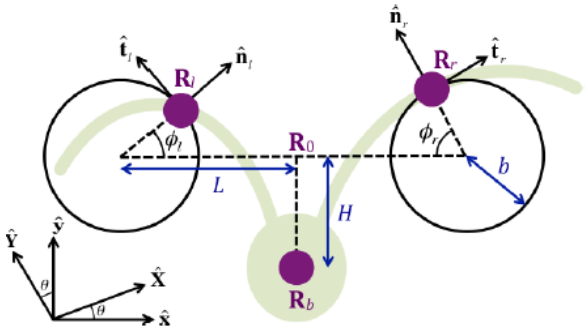

Figure 1: The three-sphere model. The two beads on the left and right represent the flagella and move around circular trajectories. The cell body is represented by a third bead. The green underlay shows a schematic of a Chlamydomonas cell.

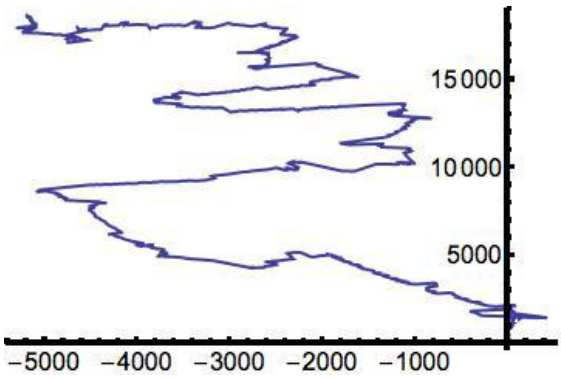

Figure 2: Run-and-tumble trajectory over ~ 1000 beat periods.

[1] Bennett, R. R. and Golestanian, R., New J. Phys. 15 (2013) 075028
[2] Bennett, R. R. and Golestanian, R., Phys. Rev. Lett. 110 (2013) 148102
[3] Polin, M., Tuval, I., Drescher, K., Gollub, J., and Goldstein, R. E., Science 325 (2009) 487

Microswimmer motility in rigid and elastic confinement

R Ledesma-Aguilar[1] and J M Yeomans[2]

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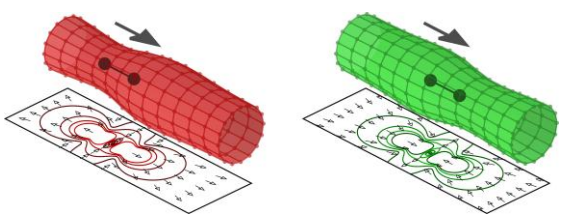
Microscopic swimmers moving in rigid and elastic confined environments are a common feature of biological systems [1]. Microswimmers, ranging from molecular motors to single and multicellular self-propelled organisms, are often faced with a world crowded by passive and active, permeable and impermeable, boundaries, such as viscoelastic gels, microtubules or cell walls. These can act as barriers or defence mechanisms against microorganisms and it has also been suggested that they can be exploited by the swimmers to enhance their motility [1].

In this work [2] we analyse the effect of confining rigid and elastic boundaries on the motility of a model dipolar microswimmer within the framework of low-Reynolds number hydrodynamics. Our model consists of a simple bead-spring dipolar swimmer confined in a mesh tube of variable bending and stretching rigidity. Numerical results show that flexible boundaries are deformed by the velocity field of the swimmer in such a way that the motility of both extensile and contractile swimmers is enhanced. The magnitude of the increase in swimming velocity is controlled by the ratio of the swimmer-advection and elastic timescales, and the dipole moment of the swimmer. We explain our results analytically by considering swimming between inclined rigid boundaries.

(a) (b)



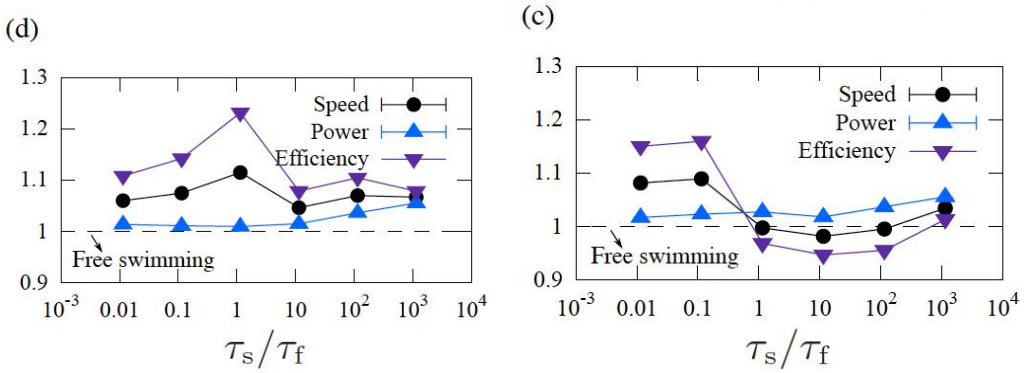


FIG. 1. (a) and (b) Numerical simulations of extensile and contractile dipolar swimmers in an elastic tube. (c) and (d) Effect of the interaction with the tube on the swimmer motility. The amplitude of the response in the swimmer speed and swimming efficiency depends on the ratio between swimmer and elastic timescales, τ_s/τ_f

[1] E. Lauga and T.R. Powers. Rep. Prog. Phys., 72:096601, 2009
[2] R. Ledesma-Aguilar and J.M. Yeomans. Phys. Rev. Lett.,111:138101, 2013

Clathrin aggregation by rotational brownian dynamics

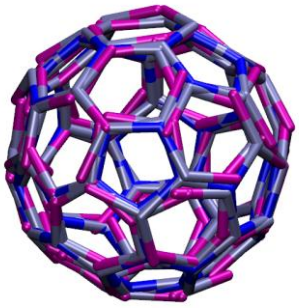
I M Ilie, W K den Otter and W J Briels

Computational BioPhysics, University of Twente, The Netherlands

The processes of endo- and exocytosis are associated with the transport of nutrients, hormones and proteins in to and out of living cells. When these molecules enter a cell, they are collected and encapsulated in vesicles for further transport to a destination within the cell. Likewise, the products of organelles are encapsulated before being transported to the edge of the cell. The central protein in the formation process of these vesicles is clathrin. Clathrins are proteins that have three long legs that enable them self-assemble into vesicles and transport cargos within the living cell.

We investigate the formation and structure of clathrin cages by means of computer simulations. To achieve this, we have developed a highly coarse-grained patchy particle model by representing a clathrin protein as a rigid triskelion with interaction sites on the legs. To simulate their dynamics, we have developed a novel Brownian Dynamics algorithm to describe the realistic motion of the protein. Our Brownian Dynamics Algorithm overcomes complications traditionally associated with rotational dynamics of anisotropic particles.

We will show results of the self-assembly of clathrin[1] into cages on a time-scale that is comparable to experimental data. In addition, the simulated cages are structurally similar to those observed by in vitro experiments and the simulations predict the clathrin interaction strength [2].



Clathrin cage obtained from Brownian Dynamics Simulations

[1] I.M. Ilie, W.K. den Otter and W.J. Briels, in preparation (2014)
[2] W.K. den Ottern and W.J. Briels, Traffic, 12 (2011)

Self-organisation of swimming bacteria in confined geometries

H Wioland[1], J Dunkel[2], E Lushi[3], F G Woodhouse[1,4] and R E Goldstein[1]

[1]DAMTP, University of Cambridge, UK, [2]MIT, USA, [3]School of Engineering, Brown University, USA, [4]University of Western Australia, Australia

Long range interactions between objects are often mediated by the surrounding fluid. In sedimenting passive colloids, for instance, particles generate flows that in turn influence their motion, leading to complex dynamics. While the same principle should apply to active suspensions of microswimmers, it has remained unclear whether explicit hydrodynamic interactions play a role in collective behaviour.

To study this problem we focus on dense bacterial suspensions for which there are known to be large-scale flows. At high concentrations, rod-like cells align at the cellular scale like liquid crystals but interactions with the surrounding medium lead to the formation of turbulent macroscopic structures such as jets and swirls.

We show that such patterns can be stabilised and controlled by confining the suspension into different geometries. Experimental work includes single vortices in flattened drops, ordering of vortex lattices into ferromagnetic-like structures and large-scale circulation in microfluidic race tracks.

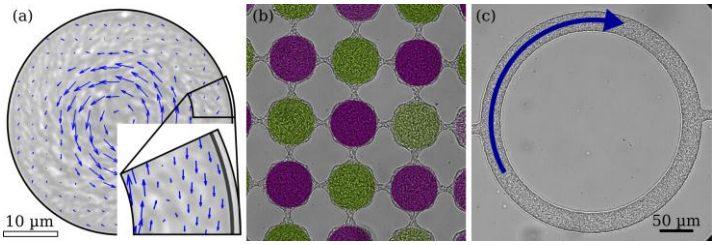


Figure: bacterial steady flows in three experimental setups. (a) Flatten drops of *B. subtilis* suspension surrounded by oil self-organizes into a single spiral vortex. (b) A lattice of vortices (coloured area, 50μm in diameter) form a antiferromagnetic pattern. Purple (resp. green) discs represent clockwise (resp. counter-clockwise) circulation. (c) A dense suspension shows spontaneous circulation in a large circular track. All experiments are done in 25μm height chambers.

Colloids and Nanoparticles

Near-wall dynamics of spherical colloids: Translational and rotational diffusion

M Lisicki[1], B Cichocki[1], S A Rogers[2], J K G Dhont[3] and P R Lang[3]

[1]Institute of Theoretical Physics, University of Warsaw, Poland, [2]Department of Chemical and Biomolecular Engineering, University of Delaware, USA, [3]Institute for Complex Systems ICS-3, Forschungszentrum Jülich, Germany

In this work, we employ Evanescent Wave Dynamic Light Scattering (EWDLS) to infer information on diffusion in a dilute suspension of Brownian particles bounded by hard planar wall, and support it by a full theoretical analysis, followed by Brownian Dynamics simulations. EWDLS is an experimental technique giving an insight into near-wall diffusion of submicron-sized particles. In such experiments, the light is scattered on colloidal particles diffusing in the presence of a wall and the scattered light intensity time autocorrelation function is measured in order to trace near-wall dynamics of a suspension. The evanescent wave which enters the sample decays as $exp(-kz/2)$ with the distance z from the wall, and restricts the scattering volume to a region characterized by the penetration depth

k^{-1}. Compared to standard Dynamic Light Scattering technique, EWDLS has some inherent features, including the effects of non-uniform illumination of the sample, and the hindrance of particles' diffusivity near a hard boundary. As hydrodynamic interactions with the wall have a pronounced effect on the dynamics of the particles on top of their direct and mutual hydrodynamic interactions, it has a reflection in the structure of scattered electric field correlation function, rendering the interpretation of experimental data much more involved.

In a dilute suspension of spherical particles, the system is fully characterised by one-particle properties. Using the Smoluchowski equation formalism, we provide a suitable theoretical framework for the derivation of exact theoretical expression for the initial decay rate (first cumulant) of the measured correlation function and relate it to the diffusive properties of the system. By using optically anisotropic spherical colloids in EWDLS experiments, and employing measurements on differently polarized light (VV- and VH-geometry) we are able to trace both the translational and rotational diffusion of spherical colloids near a wall. Moreover, our setup allows independent variation of the components of the scattering vector parallel and perpendicular to the wall, hence allowing to extract the diffusion coefficients of particles in these directions and to investigate the anisotropy of their motion in more detail.

We also present a comparison of experiments, theoretical results, and Brownian Dynamic simulations. In order to interpret the measured data, we suggest a new way of analysis to account for the long-time decay of measured correlation functions. Applying this procedure to the data, we find very good agreement between theoretical predictions and experimental results, free of adjustable parameters. This in turn gives us the possibility to measure the averaged diffusion coefficients, either translational, or rotational, and opens a new way of determining the effects of confinement on colloidal dynamics experimentally. We also develop some practical tools for experimentalists, providing them with a convenient way to calculate the first cumulant, using the expressions we have developed. The results can be directly compared with the measured initial decay rates. EWDLS seems to be the first experimental technique available to probe spatially-resolved rotational diffusion of nanoparticles in the vicinity of the wall.

[1] M. Lisicki, B. Cichocki, J. K. G. Dhont, P. R. Lang, *One-Particle Correlation Function in Evanescent Wave Dynamic Light Scattering*, J. Chem. Phys. 136, 204704 (2012)

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[3] M. Lisicki, B. Cichocki, S.A. Rogers, J. K. G. Dhont, P. R. Lang, *Translational and Rotational Near-Wall Diffusion of Spherical Brownian Particles*, submitted to Soft Matter (2014)

Asphaltene deposition in microfluidic capillary flow experiments and particulate computer simulation

C M Seifried, J P Crawshaw and E S Boek

Department of Chemical Engineering, Imperial College London, UK

Carbon dioxide (CO_2) flooding is being increasingly used for Enhanced Oil Recovery operations in depleted oil reservoirs. However, in some cases, CO_2 injection may lead to asphaltene precipitation from crude oil. Asphaltene precipitation and deposition in reservoir rocks may cause a decrease in the crude oil recovery efficiency due to reduced permeability and porosity of the reservoir rock. Asphaltene deposition is one of the costliest technical problems the oil industry has to deal with.

Despite a significant research effort, there are still limitations for predicting the asphaltene deposition in reservoir rocks. It is not yet fully identified how asphaltenes behave in reservoir rocks during laminar flow under precipitating conditions.

The microfluidic technology offers the possibility to study colloidal flow properties at low Reynolds numbers and to understand the influence of asphaltene deposition on flow properties in real reservoir rock. Thus, oil recovery rates from asphaltenic reservoirs could be optimized.

In our work, we have been studying the process of deposition from a crude oil/toluene mixture in microfluidic capillary flow experiments. This mixture is co-injected into a glass capillary with *n*-heptane, an analogue fluid for CO_2 giving rise to potential asphaltene precipitation and deposition. This enables optical observations of the deposition process using a state of the art confocal laser-scanning microscope. Simultaneously, we monitor the pressure drop as a function of time following the impact of deposition on permeability. The work builds on recent work by Boek et al. (2010) [1]. Here we extend this work by considering capillaries packed with glass beads as a more realistic approximation for flow in porous media due to reduced porosity and permeability.

We investigate the effect of flow rate and ratio of *n*-heptane/crude oil to toluene on the rate and amount of asphaltene deposition. With higher ratio, the rate of asphaltene precipitation increases, thus leading to a higher deposition rate. Deposition of asphaltenes was limited as the pressure levelled off. This suggests erosion/entrainment of deposited asphaltenes. Different flow regimes were investigated: we observe that the pressure drop increases with decreasing flow rate. Optical images (Figure 1) and experimental mass determination have confirmed that the mass of deposited asphaltenes increases with increasing flow rate, indicating that adsorption forces are dominant over hydrodynamic forces. Fluid mechanics theory and particulate simulation were used to explain these new results. The results obtained for the pressure drop measurements were confirmed by Stochastic Rotation Dynamics (SRD) computer simulations [1].

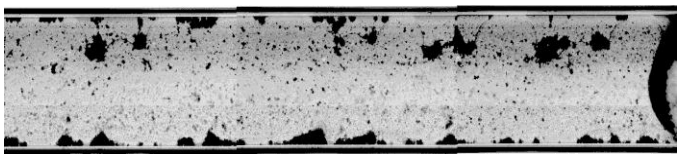


Figure 1. 3.9 mm section of a micro glass capillary with deposited asphaltenes (black spots), located near to the entrance of the capillary on the right hand side [2].

[1] Boek, E.S., Wilson, A.D., Padding, J.T., Headen, T.F., Crawshaw, J.P. (2010) Multi-Scale Simulation and Experimental Studies of Asphaltene Aggregation and Deposition in Capillary Flow, *Energy&Fuels*, 24, 2361-2368

[2] Seifried, C.M., Al Lawati, S., Crawshaw, J.P., Boek, E.S. (2013) Asphaltene Deposition in Capillary Flow, *SPE 166289*, presented at the SPE Annual Technical Conference and Exhibition, New Orleans, Louisiana, USA, 30 September – 2 October 2013

Colloidal musical chairs - String- and loop-like cooperative motion in locally perturbed 2D colloidal crystals

B van der Meer, J vd Gucht and J Sprakel

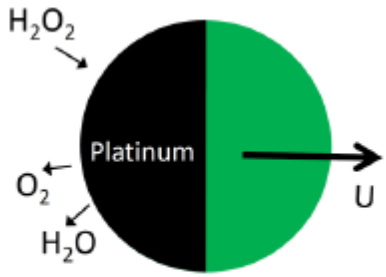
Wageningen University, The Netherlands

The application of a local or point perturbation within a crystalline solid is known to result in defect proliferation or even cause local precipitation of disordered and/or liquid phases. We study these effects experimentally in soft 2-dimensional colloidal crystals by actively driving one of the particles along the lattice axes. This local perturbation results in a rich spectrum of cooperative particle motions. Most strikingly, we observe the emergence of string- and loop-like rearrangements of particles moving in sequence. Analysis of the defect patterns suggests that these "musical chair" motions result from the unbinding and diffusion of actively generated vacancy interstitial pairs. These results shed new light on the microscopic mechanisms with which crystals can yield or melt.

How do platinum janus particles swim?

A Brown and W Poon

University of Edinburgh, UK



Platinum-polystyrene Janus particle: asymmetric reaction generates propulsion (U).

Polystyrene particles asymmetrically coated with platinum and dispersed in hydrogen peroxide solution are often used as model colloidal swimmers [1]. They swim in solution by utilising the chemical gradients produced by the hydrogen peroxide decomposing into water and oxygen. However, the precise link between the chemical gradient and the observed swimming is still not clearly understood. Previous observations are consistent with a model where the reaction propels the particle through an osmotic pressure. Simply:

$H_2O_2 \longrightarrow H_2O + 1/2\ O_2$

has more products than reactants, so there will be more molecules on the Pt side of the particle, resulting in propulsion away from that side. The previously observed direction of motion [2], and the scaling of speed with particle radius [3] and peroxide concentration [1] are consistent with this simple model.

We have found [4] that the propulsion direction can be reversed by adding an ionic surfactant. This demonstrates that the swimming mechanism is more complicated than this simple osmotic model. Further observations, of the effect of salt on swimming speed, and of the hydrogen peroxide reaction rate, also help us to rule out more complex variations of this model. We suggest, instead, that these particles swim because of ionic currents generated across their platinum surface – a generalization of the mechanism thought to propel bimetallic rods [5].

Understanding the swimming mechanism of these particles is important if they are to be used in more complex experiments, since different swimming mechanisms generate different flow fields and concentration fields around the particle. We show some preliminary experiments on the interaction of these particles with plane surfaces and colloids, which probe the hydrodynamic signature of their swimming mechanism.

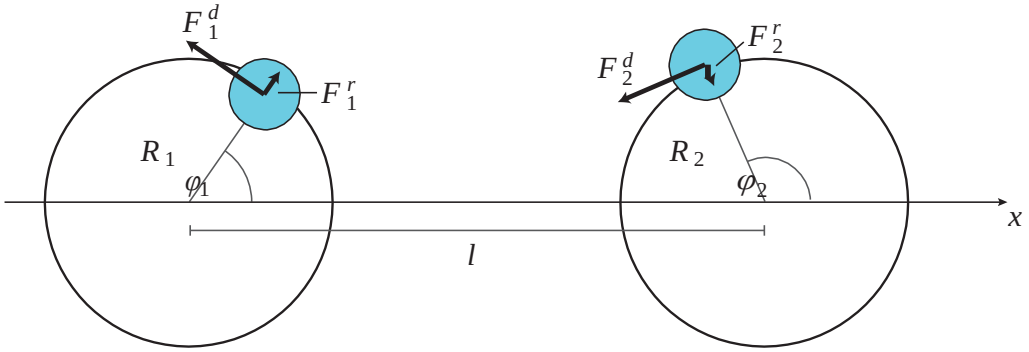
[1] Howse et al., Phys. Rev. Lett. 99, 048102 (2007)
[2] Ebbens and Howse, Langmuir 27, 12293 (2011)
[3] Ebbens et al., Phys. Rev. E 85, 020401 (2012)
[4] arXiv:1312.4130
[5] Paxton et al. J. Am. Chem. Soc. 126, 13424 (2004)

Hydrodynamic synchronisation of simple rotors

J Kotar[1], N Bruot[1], P Cicuta[1], L Debono[2], S Box[2], D Phillips[2], S Simpson[2] and S Hanna[2]

[1]Cavendish Laboratory, University of Cambridge, UK, [2]H. H. Wills Physics Laboratory, University of Bristol, UK

Hydrodynamic coupling is thought to play a role in the coordinated beating of cilia and flagella, and may inform the future design of artificial swimmers and pumps. In this study, holographic optical tweezers are used to investigate the hydrodynamic coupling between driven oscillators. In one study, the theoretical model of Lenz and Ryskin [1] is experimentally recreated, in which each oscillator consists of a sphere optically driven in a circular trajectory. The optical trap position is maintained ahead of the sphere to provide a tangential driving force. The trap is also moved radially to harmonically constrain the sphere to the circular trajectory.



Analytically, it has been shown that two oscillators of this type are able to synchronize or phase-lock under appropriate conditions [2, 3]. Here, the interplay between synchronization mechanisms is explored and good agreement is found between experiment, theory and Brownian dynamics simulations [4].

In a second study, a theoretical model is used to explore the hydrodynamic synchronisation between 2-dimensional lattices of simple rotors. In this case the rotors consist of rigid assemblies of spheres supported in an optical lattice of Laguerre-Gaussian beams. Different patterns of synchronisation are observed as the size of the lattice is varied. The symmetry of both the lattice and the rotors is also explored.

[1] P. Lenz and A. Ryskin, Physical Biology 3, 285–294 (2006)
[2] T. Niedermayer, B. Eckhardt, and P. Lenz, Chaos 18, 037128 (2008)
[3] N. Uchida and R. Golestanian, Physical Review Letters 106, 058104 (2011)
[4] J. Kotar et al, Physical Review Letters 111, 228103 (2013)

Tuesday 15 April

(invited) Capillary-driven flow in thin polymer films

K Dalnoki-Veress

Department of Physics and Astronomy, McMaster University, Canada / Laboratoire de Physico-Chimie Théorique, France

The physics of soft materials is distinct from hard matter as the weaker intermolecular bonds can result in a large response to external stresses. A surprising aspect of these materials is that at interfaces and on small lengthscales, like thin films or coatings, these materials can have properties that differ vastly from those of bulk systems. The difference can be the result of molecules being confined or because the interface plays a greater role the smaller the size of the system studied. In this talk I will summarize our recent work on using “stepped films” to uncover some of the physics relevant to polymer rheology on length scales comparable to the size of polymer molecules. The work presented will focus on the efforts of a larger collaboration (Élie Raphaël's theory group [1], James Forrest’s experimental group [2], and the experimental group at McMaster [3]). The simple geometry of a polymer film on a substrate with a step at the free surface is unfavourable due to the excess interface induced by the step. Laplace pressure will drive flow within the film which can be studied with optical and atomic force microscopies. These studies provide an opportunity to study how systems transition from the bulk to confined. Starting with some of the results of levelling experiments on simple stepped films as well as the levelling of polymer droplets on thin films (see figure), I will finish with a discussion on our more recent efforts to elucidate confinement effects.

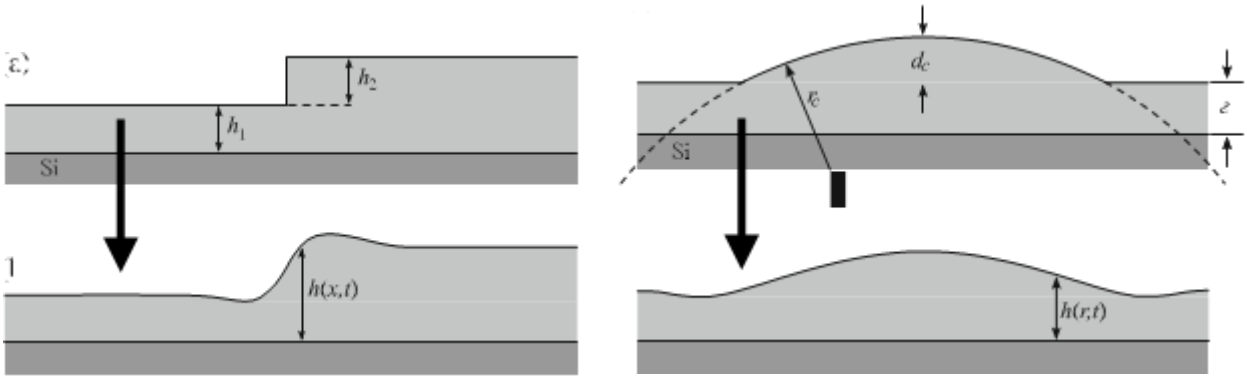


Figure: Schematic of the systems studied. Either a stepped film (left) or spherical cap placed atop an identical film (right) is prepared in the glassy state. Upon annealing above the glass transition such films flow, driven by the Laplace pressure and mediated by viscosity.

[1] T. Salez, M. Benzaquen, E. Raphaël, Gulliver Laboratory, CNRS-ESPCI, Paris, France
[2] Y. Chai & J. A. Forrest, University of Waterloo, Waterloo, Canada.
[3] J. D. McGraw, O. Bäumchen, S. L. Cormier, P. D. Fowler, M. Backholm

Polymers, Polyelectrolytes and Biomolecules

Unwinding dynamics of polymers: a model for single biomolecules?

J-C Walter

University Montpellier 2, France

The relaxation dynamics of a polymer wound around affixed obstacle constitutes a fundamental instance of polymer with twist and torque and it is of relevance also for DNA organisation and transcription of DNA into RNA. After an introduction on polymer physics and static properties of the winding of a polymer, we present our results on the unwinding dynamics by means of simulations and Langevin equation analysis. The latter predicts a relaxation time scaling as a power of the polymer length times a logarithmic correction related to the equilibrium fluctuations of the winding angle. The numerical data support this result and show that at short times the winding angle decreases as a power-law. This is also in agreement with the Langevin equation provided a winding-dependent friction is used, suggesting that such reduced description of the system captures the basic features of the problem. Moreover, we give a quantitative description of the existence of two regimes during the relaxation and a split of the polymer between two parts: a helical part and a random coil.

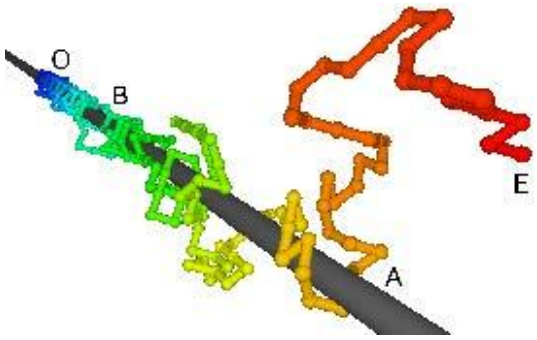


Figure 1: Unwinding process of a polymer: initially, the polymer if fully wound around a bar in a helical configuration with one end attached and the other end free. The relaxation proceeds through the rotation of the free end around the bar with an increasing coil. We give a quantitative description of this process: two regimes at short and large time, and in each of these regimes a split of the polymer between a helical part and a random coil. This model suggests possible applications for the description of biomolecules (namely DNA organisation and transcription).

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[2] *Unwinding dynamics of a helically wrapped polymer* in preparation Walter J-C, Baiesi M, Carlon E & Schiessel H (2014)

Threading dynamics of ring polymers in a gel

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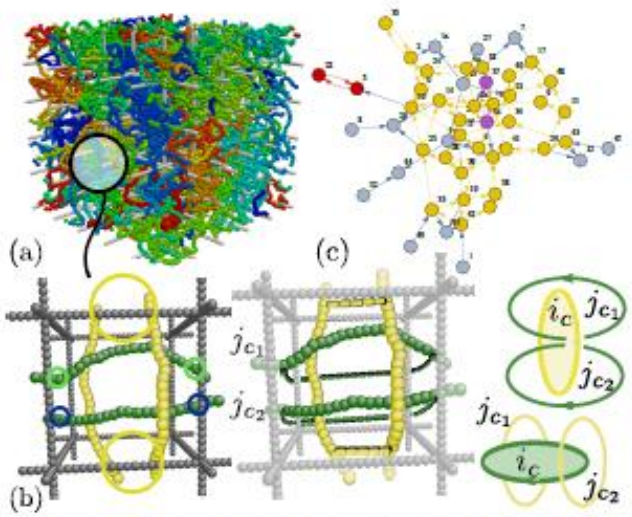
[1]Complexity Science DTC, University of Warwick, UK, [2]Department of Physics, University of Edinburgh, UK, [3]Department of Physics, University of Padua, Italy



(a) Snapshot of our system. (b) Snapshot of the threading of two chains indicating the closure construction that we employ for threading detection. (c) Snapshot of the directed network of inter-penetrating rings.

Ring polymers continue to present a challenge to the theoretical community as the polymers lack of ends represents a severe topological constraint on their conformations, especially when diffusing through a gel. In particular, threadings between rings have always been conjectured to play an important role in solutions of closed chains, from the work of Klein (Klein, Macromolecules 118 (1986)) to more recent ones (Halverson et al, J. Chem. Phys. 134 (2011)), but always proved very hard to detect and quantify. We performed large-scale Molecular Dynamics simulations of a concentrated solution of unknotted, unlinked rings in a background gel made up of a three dimensional cubic lattice of static polymer segments with lattice spacing equal to the chains Kuhn length (Fig. (a)), in order to detect inter-ring penetrations. We took advantage of the ordered architecture of our gel to unambiguously identify inter-ring threadings by measuring the linking of closed curves (Fig. (b)). We show that some of threadings have a life-time that is at least comparable to that of the longest relaxation time of the chains and argue that they may be much longer for longer chains than those we were able to simulate here. The achievement of an adequate description of inter-ring interactions could explain most of the confusion on the macroscopic properties of solutions of rings, where, on top of a fast diffusion, one can observe very long lived correlations. Finally, we compare our system to an evolving (directed) network of penetrating rings (Fig. (c)) and suggest that, in the limit of very long chains, a spanning connected component of threading rings may emerge, which would then exhibit very slow (glassy) dynamics at the scale of centre of mass motion for each chain, while retaining substantially unhindered motion at the level of individual chain segments. Having observed that the number of threadings per chain grows linearly with the length of the rings, we conjecture that such a topological glass is bound to emerge in the limit of very long rings.

New method to predict the surface tension of complex synthetic and biological polyelectrolyte/surfactant mixtures

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While the surface tension of complex mixtures determines the fate of important natural processes like the stability of aerosol droplets in clouds and the biological function of lung surfactants, the property is notoriously difficult to interpret and model. For example, it was established over a decade ago that some strongly interacting polyelectrolyte/surfactant (P/S) mixtures exhibit a striking cliff edge peak in their surface tension isotherms [1]. Recently we have systematically linked the surface tension peak of a strongly interacting P/S mixture to slow dynamic changes in its bulk phase behavior [2], and we went on to demonstrate the non-equilibrium nature of the system [3]. Here we announce a simple new approach that successfully predicts the surface tension of two synthetic (Pdadmac/SDS and NaPSS/DTAB) and one biologically-relevant (DNA/DTAB) mixtures [4]. The approach

is based on the non-equilibrium framework of comprehensive precipitation of kinetically-trapped aggregates followed by their transport under gravity away from the probed interface. Importantly our approach does not need any measurements of the surface properties of the mixtures; only the surface tension isotherm of the pure surfactant and some bulk measurements of the mixtures are required. This simplification in our understanding of the surface properties of strongly interacting mixtures may lead to the optimization of a broad range of applications involving commercial synthetic polymers, DNA and proteins at surfaces, such as in common household formulations and rapidly expanding research areas such as targeted drug and gene delivery.

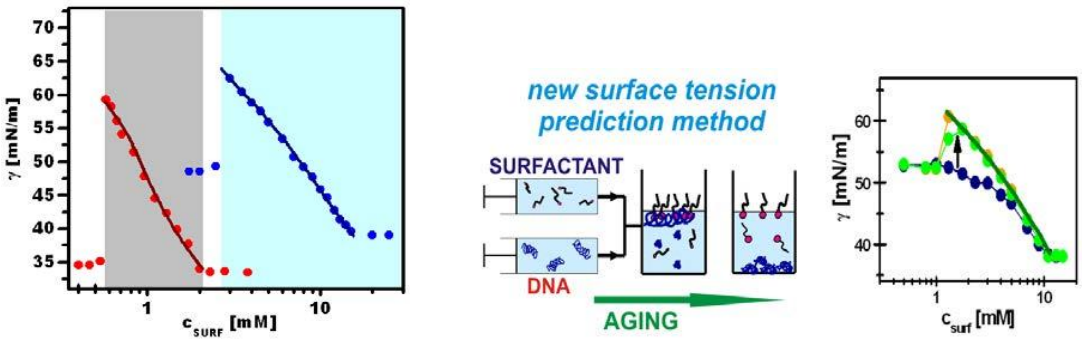

Figure. Left. Surface tension of aged Pdadmac/SDS (red) and NaPSS/DTAB (blue) solutions with our predictions of the surface tension which are not based on any surface measurements of the mixtures; shaded area indicates the phase separation regions. Right. Table-of-contents image from our recent letter in *Langmuir* [4] showing the prediction for aged DNA/DTAB mixtures.

[1] Staples, E.; Tucker, I.; Penfold, J.; Warren, N.; Thomas, R. K. Organization of polymer–surfactant mixtures at the air–water interface: sodium dodecyl sulfate and poly(dimethyldiallylammonium chloride). *Langmuir* 2002, *18*, 5147–5153

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[3] Campbell, R. A.; Arteta, M. Y.; Angus-Smyth, A.; Nylander, T.; Varga, I. Effects of bulk colloidal stability on adsorption layers of poly(diallyldimethylammonium chloride)/sodium dodecyl sulfate at the air-water interface Studied by Neutron Reflectometry. *J. Phys. Chem.* B. 2011, 115, 15202–15213

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Kinetic control over out-of-equilibrium self-assembled hydrogels

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Self-assembly under thermodynamic control gives a well-defined single state due to minimizing the Gibb's free energy. In contrast, kinetic control over self-assembly processes allows us to access many different states of a system. However, our limited understanding of the kinetics of self-assembly process restricts our ability to design kinetically controlled self-assembly routes. Here we explore a new method to kinetically control multi-step self-assembly using dynamic combinatorial chemistry. The first step starts with a dynamic combinatorial library of macrocycles functionalised with different numbers of peptide side-groups. The macrocycles are held together by reversible disulfide covalent bonds. Then the peptides start to interact to assemble macrocycles into fibres, which form a hydrogel. We tune the physical properties of the hydrogel using various methods such as photo-irradiation, adding cross-linker and varying salt concentration. We relate the gel properties to their structure by performing rheology measurement and direct visualization techniques including Cryo-TEM and AFM. Our results suggest that, on

one hand, photo-irradiation initiates a reshuffling of the disulfide bonds within the fibres, causing the fibres to be less fragile and including gelation through entanglement of the fibres. On the other hand, adding cross-linker or varying salt can enhance the gel strength significantly. These results open up new possibilities in the kinetic control of self-assembly process.

Self-Assembly, Biomimetics and Pattern Formation

Enzyme-driven chemotactic synthetic vesicles

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The movement of organisms toward (or away from)[1] specific chemicals in their environment is possibly one of the most important evolutionary milestones for many living systems to secure a superior position over non motile competitors. In particular, chemotaxis is a very important biological process used by many unicellular organisms to gather food and/or escape danger[2] as well as by multicellular system to control tissue development[3], immune response[4] and cancer metastasis[5]. From a physical point of view, chemotaxis is possibly the longest ranged form of chemical targeting extending over several orders of magnitude larger than the motile organism itself.[6] Here we report for the first time an example of nanoscopic chemotactic system fully driven by enzymatic conversion of small water soluble molecules. We demonstrate this by encapsulating enzymes into nanometer sized synthetic polymeric vesicles also called polymersomes. These polymersomes are formed by double-layered membranes that are topologically designed to contain permeable domains within an impermeable matrix. The asymmetric distribution of these permeable domains enables to direct and focus the discharged enzymatic reaction products generating thrust. This in turn allows propulsion with direction controlled by the substrate concentration. The combination of membrane topology and enzyme encapsulation is a new approach, which produce chemotaxis without the need of chemical modification. We demonstrate this by using physiologically-relevant hydrogen peroxide and glucose coupled with catalase, glucose peroxidase and their combination loaded within asymmetric polymersomes. This can be potentially applied into several biomedical applications spanning from targeted delivery to biochemical sensing. Finally, we propose a new mechanism of advanced diffusion controlled by the vesicle membrane topology suggesting the role of selective permeability as potential new way to produce nanoscale locomotion.

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[3] VanHook, A. M. Focus issue: organ development from beginning to end. *Science signaling* 1, eg10, doi:10.1126/scisignal.149eg10 (2008)

[4] Swaney, K. F., Huang, C. H. & Devreotes, P. N. Eukaryotic chemotaxis: a network of signaling pathways controls motility, directional sensing, and polarity. *Annual Review of Biophysics* 39, 265-289, doi:10.1146/annurev.biophys.093008.131228 (2010)

[5] Roussos, E. T., Condeelis, J. S. & Patsialou, A. Chemotaxis in cancer. *Nat Rev Cancer* 11, 573-587, doi:10.1038/nrc3078 (2011)

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Encapsulating hydrogenase active site analogues in peptide-based supramolecular hydrogels: a photochemical study

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Synthetic inorganic compounds inspired by the active site of the hydrogenase (H_2-ases) enzymes have attracted much scientific attention as a result of their ability to catalyse the reversible reduction of protons to form dihydrogen. It is anticipated that these systems will ultimately offer a more economic and renewable alternative to the platinum-based approach currently used in fuel cells. These bio-inspired compounds are however limited in terms of technological applications by oxygen sensitivity and a reduced catalytic rate in comparison to the native enzyme. In an effort to address some of these issues we have incorporated hydrogenase model compounds (e.g. Fig. 1(a)) into low molecular weight (LMW), peptide based, hydrogels that are able to modify both the chemical stability and photochemistry of the encapsulated molecule, offering potential new routes to exploitation of these systems.[1]

LMW hydrogelators, and in particular self-assembled oligopeptide-based gels, have shown great potential in encapsulating enzymes with retention or improvement of catalytic activity.[2] These materials are generally low-cost, biocompatible and highly tuneable. We have successfully incorporated a range of [FeFe]-H_2-ase active site mimics into Fmoc-dipeptide hydrogels containing only 1% gelator in aqueous environments (Fmoc = 9-fluorenylmethoxycarbonyl, Fig. 1(b)). Fourier transform infrared (FTIR) and UV_{pump}-IR_{probe} time-resolved infrared spectroscopy (TRIR, Fig. 1(c)) experiments have been carried out and both show results that differ with respect to data obtained in the solution phase. Both FTIR and TRIR experiments show results that are consistent with an immobile, but strong hydrogen bonding environment in the gel phase that restricts dynamic processes such as photo-induced isomerisation while maintaining the fast vibrational relaxation rates observed in solution,[3] confirming the gel's unique properties. In addition, the chemical stability of the encapsulated species was observed to be improved relative to solutions.

In summary, encapsulating hydrogenase active site mimics in LMW hydrogels induces significant changes in their photochemistry and chemical stability. Since understanding and ultimately controlling the mechanistic role of ligands near Fe centres is likely to be crucial in exploiting artificial hydrogenases, these gels may offer a new option for future materials design involving catalysts.

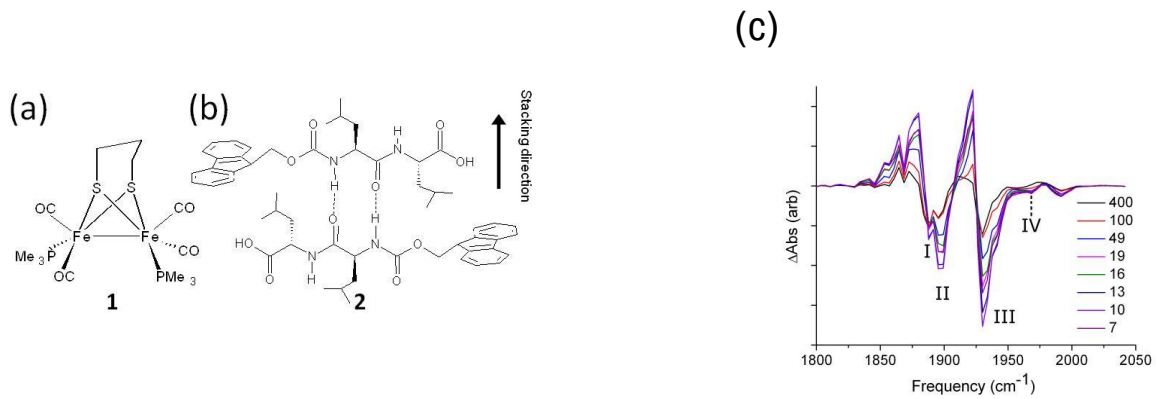

Fig. 1. (a) Chemical structure of one of the H_2-ase active site mimics studied. (b) Chemical structure and schematic diagram of the β-sheet-type stacking of the peptide-based gelator (Fmoc-Leu-Leu). (c) TRIR difference spectra of the hydrogenase-inspired model compound shown in (a) encapsulated in a peptide hydrogel (b). The data range shown corresponds to UV_{pump}-IR_{probe} time delays of 1-400 ps.

[1] Frederix, P. W. J. M.; et al. *Dalton Trans.* 2012, *41*, 13112–13119
[2] Gao, Y.; et al. *Chem. Soc. Rev.* 2010, *39*, 3425–3433
[3] Kania, R.; et al. *J. Chem. Phys.* 2012, *136*, 044521–044521–9

Motility-induced phase separation in an active dumbbell fluid

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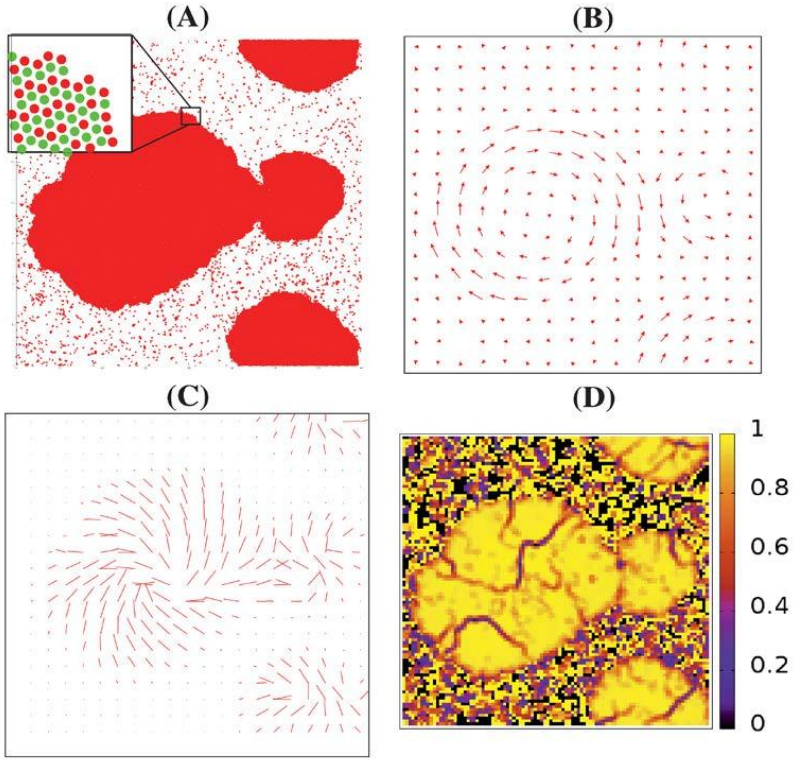
We study a suspension of active dumbbells of variable density, as a minimal example of an active polar fluid. As in a fluid of spherical swimmers, we find that motility triggers a non-equilibrium phase separation if the density exceeds a critical threshold. We also show that the phase separation is lost when the active force becomes too large, ultimately due to inertial effects. Unlike their spherical counterparts, the aggregates which assemble spontaneously break chiral symmetry and rotate; they also display a nematic ordering with spiral patterns. An example of such an aggregate is given below.



(A) Snapshot of a phase-separated active dumbbell fluid with three clusters (two of which are touching). The inset shows a detail of the dumbbell configuration; red and green beads indicate the tail and head of the dumbbells respectively. (B) Coarse grained velocity field corresponding to the snapshot in (A). (C) Coarse-grained orientation profile of the dumbbell fluid (P) corresponding to the configuration in (A). (D) Hexatic order parameter corresponding to the configuration in (A).

Atom-scale computer-aided design of organic-inorganic interfaces

D Thompson

Department of Physics & Energy and Materials and Surface Science Institute, University of Limerick, Ireland

In this talk I will discuss the difficulties in controlling nanoscale physics and describe how atomic scale computer simulations can aid experiments in the design of functional organic-inorganic interfaces. I will present recent results on experimental/simulation co-design of ferrocene-alkanethiolate self-assembled monolayer (SAM) films on silver; these films exhibit an atom-level sensitivity in their electrical properties.[1] I will also describe combined experiments and simulations of controlled motion of dendrimer molecules on carbohydrate-functionalised SAMs[2] and present the synthesis and interlinking of dendrimer-wrapped gold nanoparticles.[3]

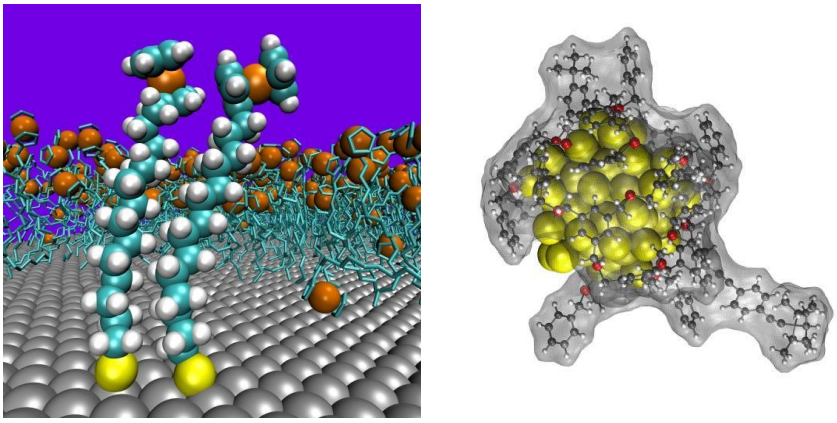


Figure 1. (left) Ferrocene-alkanethiolate molecules with an odd number of alkyl carbon atoms stand tall on silver and form close-packed SAMs that block leakage currents in molecular diodes. [1] (right) Gold clusters stabilised by thioether dendrimer molecules provide building blocks for future molecular electronic devices. [3]

[1] N. Nerngchamnong, Y. Li, D. Qi, L. Jian, D. Thompson and C.A. Nijhuis, *Nature Nanotechnology*, 2013, 8, 113

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Biological Systems

The role of intrinsically disordered proteins under conditions of abiotic stress

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University of Cambridge, UK

The ability of extremophile organisms to survive hostile conditions has caused us to reassess the requirements for life. LEA proteins are linked to the acquisition of cold and desiccation tolerance in plants and animals. As intrinsically disordered proteins (IDPs), LEA proteins are inherently tolerant to stress-induced denaturation, and LEA proteins have been shown to protect globular proteins, such as pig heart citrate synthase (CS) and rabbit muscle lactate dehydrogenase, and a human cell proteome from abiotic stresses [1]. The mechanism by which LEA proteins protect folded proteins is still unclear. There are several hypotheses regarding the mechanism behind the protective abilities of LEA proteins. Leading models include chaperone- and shield-like interactions. However, our preliminary work through aggregation assay, isothermal titration calorimetry, dynamic surface tension and small angle neutron scattering experiments, suggests that bulk interaction mechanisms are insufficient to fully explain the observed LEA protein's aggregation protection of CS and has led us to propose an additional protection mechanism: the preferential adsorption of LEA proteins at air/water interfaces. Unlocking the mystery of IDPs and their role in extremophile survival mechanisms will be beneficial in the development of new technologies for preserving biological materials.

[1] S. Chakrabortee, C. Boschetti, L. J. Walton, S. Sarkar, D. C. Rubinsztein and A. Tunnacliffe, *PNAS*, 2007, 104, 18073-18078

Traffic jams on the microtubule network

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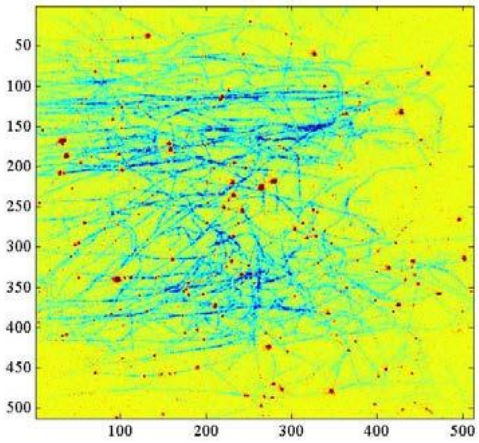
The transport of organelles and proteins is of vital importance for living cells. Besides passive transport by diffusion, active transport by moleculair motors hopping over the cytoskeleton is crucial for the survival of cells. We study *in vitro* the movement of moleculair motors over microtubule network. With Totally Internal Reflection Microscopy (TIRF) we image the 2D network of microtubules and the motors moving over the network simultaneously (see Figure). Traffic jams of moleculair motors seem to form at the intersection of microtubules in the network. The rate at which motors approaching a crossing continue along the same microtubule or switch to the other microtubule appears determining for the transport along the network.

We combine this experimental study with numerical simulation of particles hopping over a netwrok. We use the Totally Assymetric Exlusion Process (TASEP), a paradigmetic model for nonequilibrium transport, to model the dynamics along the microtubules. From preliminary numerical work, indeed the dynamical rules at the intersection of the network seem to be the key factor for the formation of traffic jams along the microtubule segments



A TIRF image of the microtubules (blue) and kinesin motors (red)

Multiscale self-assembly of fibrin governs its polymerization kinetics, fiber and network structure, as well as nonlinear rheological properties

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Fibrin is a fibrous biopolymer that forms a tough three-dimensional mesh and clots the blood in a wound site. This network needs to be sturdy yet extensible under shear to sufficiently protect the area during healing. At the same time, the structure of the self-assembled network needs to be precisely controlled to allow timely breakdown of the clot, which could otherwise present thrombotic complications. Studying the structure and mechanics of fibrin clots is therefore important not only in understanding the molecular origins of their behavior and regulation in various diseases, but also in designing hemostatic materials, particularly in surgical settings.

By monitoring and analyzing the scattering of self-assembling fibrin gels, we identified different temporal stages in which fibrils aggregate laterally to form floppy fibers, followed by slow compaction of the fibers. These stages are reflected in the fast (10 min) and slow (hours) development of the elastic modulus. Furthermore, we have found that fibrin gels stiffen nonlinearly with stress, and comparison to theoretical model reveals that the stiffening

regimes are linked to the different deformation modes at fiber and network levels. Interestingly, the rheological response shows multiple plateau-stiffening steps, a behavior unique to fibrin gels. Moreover, the presence of Factor XIII, a natural cross-linker of fibrin, is found to alter both the polymerization kinetics and time-dependent rheological response. However, the behavior of uncross-linked and cross-linked gels collapse onto a single curve at large stresses, suggesting that single fibril mechanics dominates at large deformations. By combining rheological studies with microstructural characterization using microscopy and turbidity measurements, we propose a model to explain how the hierarchical structure of fibrin network is interconnected with its mechanics at multiple length- and time-scales.

Nanoscale ligand spacing influences receptor triggering in immunological synapses

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[1]Department of Materials, Imperial College London, UK, [2]Division of Cell and Molecular Biology, Imperial College London, UK, [3]Skirball Institute of Biomolecular Medicine, NYU School of Medicine, USA, [4]Department of Biostatistics, NYU School of Medicine, USA, [5]Kennedy Institute of Rheumatology, University of Oxford, UK, [6]Manchester Collaborative Centre for Inflammation Research, University of Manchester, UK

Immunological synapses, domains of close adhesive intercellular contact, play a crucial role in key decision-making processes in the immune system. By creating a stable connection, they enable immune cells to integrate signals from a complex range of ligand molecules on the surfaces of target or information-bearing cells. Such processes enable the immune system to distinguish harmless molecules and cells from those that pose a threat, and are of vital clinical interest in infection, cancer and autoimmune disease [1].

Here, we create biomimetic ligand nanoarrays that actively control the spatial distribution of cell surface molecules in a model immunological synapse. By using these to stimulate immune cells we show that this spatial distribution acts directly to determine the outcome of the decision-making process. The nanoarrays were formed from gold nanospheres with controlled interparticle spacing in the range 25–104 nm [2]. These were biofunctionalized with ligand molecules that stimulate activating receptors on T cells and natural killer (NK) cells. In both cases, the strength of response decreased strongly with increasing spacing, falling to background levels by 69 nm in the T cell system and 104 nm for the NK cell system [3]. These results demonstrate that immune receptor triggering is influenced by the nanoscale spatial organization of receptor/ligand interactions.

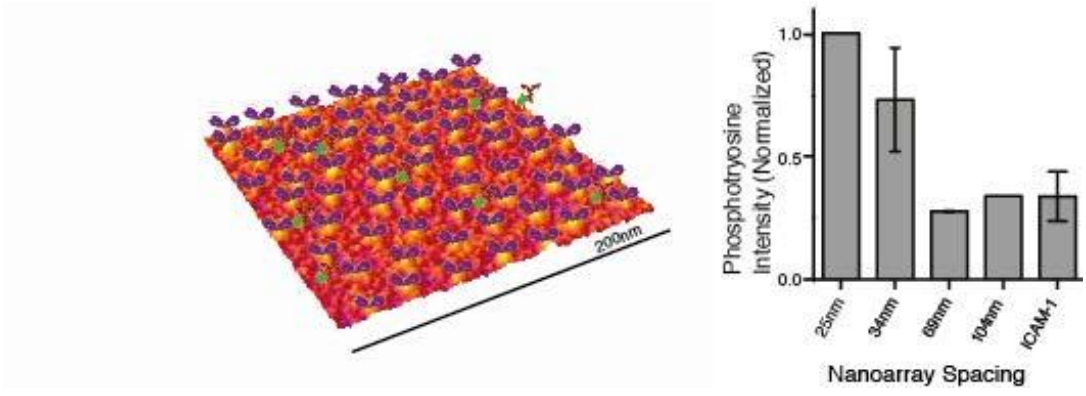

Fig. 1. (Left) T cell activating nanoarray formed by functionalizing a gold nanoparticle array with T cell-binding proteins and antibody fragments. The figure shows structures of immobilized proteins superimposed on a 3D plot of a scanning electron micrograph of a representative gold nanosphere array, with T cell stimulating $F(ab')_2$ fragments shown in purple, cell adhesion ligands in red and streptavidin used for functionalization in green. (Right) Dependence of T cell early stage activation signaling, indicated by phosphotyrosine intensity, on the spacing of stimulating nanoarrays.

[1] Xie *et al.*, *Immuol. Rev.*, 251, 65 – 79 (2013)
[2] Calvacanti-Adam *et al., Biophys. J.*, 92, 2964 – 2974 (2007)
[3] Delcassian *et al., Nano Letters*, 13, 5608 – 5614 (2013)

Exploring the molecular bases of cytoskeleton-cell membrane interactions, by live imaging approach

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Cellular architecture and compartmentalisation are organised as bi-dimensional fluid membranes, which are assembled by essential molecules for the life of a cell: the phospholipids. These are not just crucial for the cell membranes formations, since they also play a pivotal role in the formations of "raft" domains at the membrane level[1], together with the action of proteins. In addition, they participate in several other fundamental cell mechanisms including proteins regulations, vesicular trafficking, and cell motility[2].

Over the last years, many cellular processes have been deeply characterised, especially from a molecular biology and biophysics viewpoints. However, cell membrane dynamics still represent one of the most complex process yet to be fully elucidated. This is due mostly due to a general lack of technologies suitable in lipidomic investigations. In fact, bio-molecules such as phospholipids, ceramides, and sterols cannot undergo genetic modifications, and hence being then analysed in live cells using traditional fluorescence protein approaches.

In this work, we used polymersomes as synthetic self-assembled delivery system[3], to achieve a stable and optimal distribution, in live cell, of five different membrane and cytoskeleton probes: BODIPY®Phosphocholine (PC), NBD-Cholesterol (NBD-C), BODIPY®TB-Ceramide (BC), TopFluor®PI(4,5)P2 (PIP2) and Phalloidin-ATTO647 (PHAL). The effective delivery and the topological membrane-distributions of these probes were evaluated in mouse embryonic fibroblast (NIH-3T3 cell line). The results showed an efficient delivery for all the tested probes in live cell.

Furthermore, it was possible to characterize the specific interplay and overlap between the different lipid domains in diverse cell membrane areas, by means of confocal analyses. Moreover, the delivery of PHAL polymersomes enabled a clear staining of F-actin in live cell, without causing any toxicity.

Using such an approach, we have been able to elucidate the cooperation between PIP2 domains and cytoskeleton during sophisticated cellular mechanisms such as adhesion, polarization, and spreading process, showing a peculiar phosphatidylinositol active transportation to the membrane protrusion. In conclusion, this work enables to reach a better understanding of the complexity of lipid organization, and provides important explanation about the interplay that subsists between these bio-molecules and the F-actin network in live cell.

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Rheology and Non-equilibrium Phenomena

Length-scale dependent aging and plasticity of a colloidal polycrystal under cyclic shear

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Most solids like metals and ceramics are polycrystals, i.e. aggregates of crystalline grains separated by 2D defects, the grain boundaries (GBs). Although GBs sliding is believed to be involved in the irreversible deformation (plasticity) of polycrystalline solids, the microscopic mechanisms at play are still poorly understood. We propose a colloidal analog of atomic polycrystals obtained by doping a copolymer micellar crystal with nanoparticles (NPs) [1,

2]. During the crystallization NPs are partially expelled from the lattice and segregated into the GBs allowing one to probe their structure with microscopy (fig.1) or light scattering.

We investigate plasticity in the colloidal polycrystal by using confocal microscopy (fig.2) and time-resolved light scattering performed using a novel light scattering apparatus [3] specifically designed to access the dynamics of the GBs at different q vectors. We follow the evolution of the GBs network as the sample is submitted to a large number of shear deformation cycles. The dynamics associated with plasticity are found to be ballistic (fig.3a) and to slow down until a steady state is reached after a large number of shear cycles.

Surprisingly, the cross-over time between the initial aging regime and the steady state decreases with increasing probed length scale (fig.3b), hinting at a hierarchical organization of the GBs dynamics.

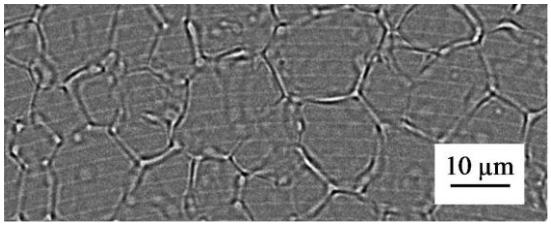

Fig.1: light microscopy image of the GB network of a colloidal polycrystal doped with nanoparticles.

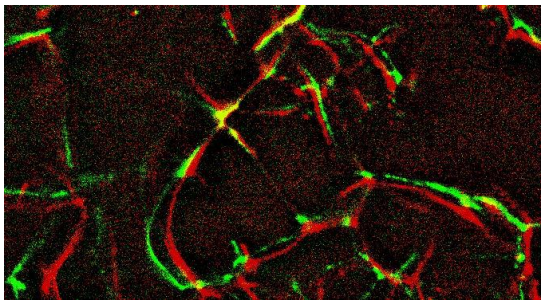

Fig.2: overlay of two confocal images of the GB network taken after 1 (red) and 2617 (green) shear cycles. The images overlap perfectly the zone highlighted by the white circle. However, in most of the field of view, the GB network does not overlap, revealing an evolution of the polycrystalline microstructure.

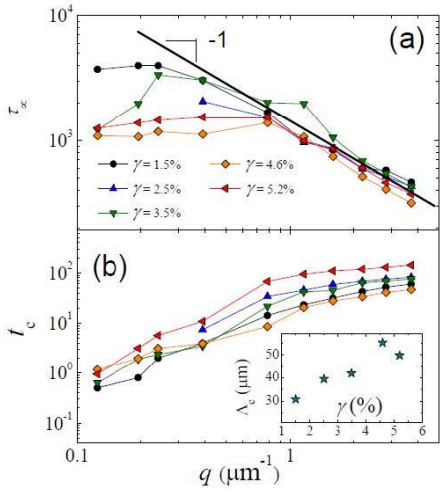

Fig3: (a) q dependence of the relaxation time of the steady state showing that the dynamics associated with plasticity is ballistic. (b) q dependence of the crossover time between the initial aging regime and the steady state. The cross-over time decreases with increasing probed length scale. Data are labelled by the strain amplitude, as indicated in the legend.

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Particle response during the yielding transition of colloidal glasses

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Yielding is central to the relaxation, flow and fracture of a wide range of soft and molecular glasses, but its microscopic origin remains unclear. Here, we elucidate the yielding of a colloidal glass, silica particles 50nm in diameter, by using x-ray scattering (at DESY facility, Hamburg) to monitor the structure factor during the yielding process. We apply a recently introduced combination of vertical small-angle x-ray scattering and rheology [1] to the

oscillatory shear measurements (see figure 1 left), and follow the structure factor evolution during the increasing strain amplitude. Surprisingly, we observe a sharp transition at critical strain $\gamma_0^\star$ in the orientational ordering of the nearest-neighbour structure upon yielding, in contrast to the smooth variation of the viscoelastic moduli (see figure 1 right). This transition is accompanied by a sudden change of intensity fluctuations towards Gaussian distributions. Interestingly the crossing point of the viscoelastic moduli occurs close to $\gamma_0^\star$, allowing us to associate the sharp structural transition with the rheological yielding of the material. Even during the reverse transition, i.e. from large to small strain amplitude the structural transition at $\gamma_0^\star$ happens close to the intersection of the moduli, with almost no hysteresis. We thus identify yielding as a new, dynamically induced transition of the glass in response to the applied shear [2].

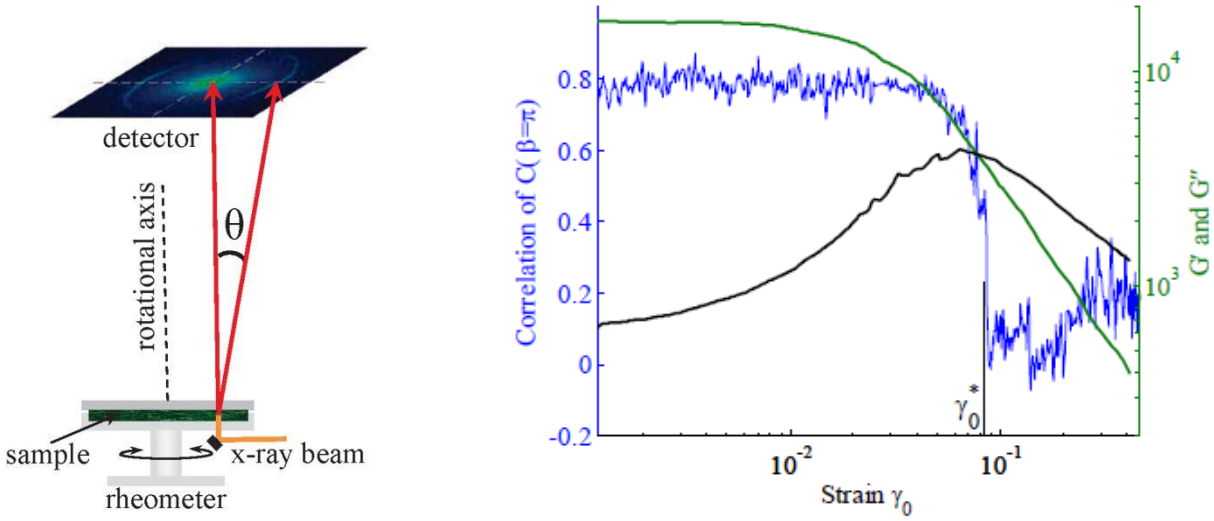

Figure 1. Left: Schematic of the experimental setup showing the x-ray beam and detector with respect to the rheometer and the layer of sheared suspension. The rheometer is stress controlled and we use plate-plate geometry. The x-ray beam passes through the suspension at 0.78 times the disc radius; the beam diameter is smaller than 0.1 mm, much smaller than the disc radius of 18mm. Right: Nearest-neighbor orientational order parameter $C(\beta = \pi, \gamma_0)$ as a function of strain amplitude γ_0 (left axis, blue curve). Also indicated are the elastic and viscous moduli, G' and G" (right axis, green and black curves).

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Molecular dynamics simulations of flow in nanopores

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A no-slip boundary condition is usually assumed when estimating the velocity of fluid in a channel of continuum flow dimensions. However, at the nanoscale, molecular roughness has a large impact on fluid behavior at surfaces and in pores [1]. With increasing roughness, the no-slip boundary condition arises naturally. However, at lower fluid densities slip appears [2]; a non-zero velocity arises at the wall of the channel. If slip is not taken into account then the mean velocity in the channel can be underestimated dramatically. This can be a problem when dealing with flow in porous structures where the nanoporosity is non-negligible, such as engine deposits and gas shales. Quantifying the amount of slip in a channel of given material-fluid combination is a challenge that requires simulation techniques such as Molecular Dynamics (MD). However, MD is limited to relatively small simulation boxes, commonly only a few nanometres. As such, there is a need for a procedure for calculating flow in nanopores for larger geometries than just single pores.

This study is specifically aimed at understanding transport of hydrocarbons in nanoporous engine deposits. Engine deposits are complex carbonaceous materials accumulating on the inner surfaces of car engines that can act as a “sponge” and adsorb fuel components [3]. The presence of these deposits may lead to adverse engine performance such as power loss, slow acceleration, poor drivability, a poor cold start and increased emissions. The mechanisms strongly depend on the porous nature of the deposits and may or may not depend on the surface roughness of pores. A previous study found that the equilibrium adsorption capacity is certainly sufficient to perturb the combustion process, however a method is needed for finding credible adsorption within a realistic time frame, i.e. that of an engine cycle (circa 1 ms).

Equilibrium [5] and non-equilibrium Molecular Dynamics (MD) are used to study slip within slit pores. An MD package known as GROMACS [4], primarily designed for biomolecular systems such as proteins and lipids, is used here. The effects of the solid surface structure, wettability and method of restraining the surface on the observed slip length are investigated as well. The study is then extended to include the effect of surface geometry on the relation between the planar slip length and slip velocity and a model produced based on the surface curvature. Furthermore, surface roughness is quantified and included in the model. Finally, the geometry dependent model for slip is implemented as a boundary condition in a multi-phase multi-component Lattice Boltzmann (LB) code, for simulating flow in larger scale systems such as the porous structures that exist in engine deposits. LB method is an efficientsolution for simulations of complex flow in porous media, due to its statistical physics background, easy implementation, strength of dealing with complex geometries and inherent parallelism [6]. The LB code is then validated against MD simulations on complex geometries.

With adaptations implemented within the LB model and the model validated, MD simulations are performed on surfaces representative of engine deposits in order to extract slip lengths for use in LB. Future work will include imaging these carbonaceous deposits for use as geometries in the model, for flow and spontaneous imbibition calculations.

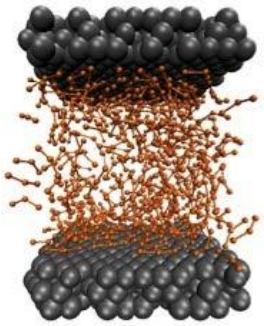

Figure 1: Snapshot of model nano-pore in MD simulation

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Microfluidic-SANS: in situ molecular insight into non-equilibrium phenomena in complex fluids

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The coupling of microfluidics and small angle neutron scattering (SANS) is successfully demonstrated for the first time. We have developed novel microdevices with suitably low SANS background, high pressure and chemical compatibility for the investigation of flow-induced phenomena and phase mapping of complex fluids. We successfully obtained scattering profiles from as low as 50 micron channels, in 1s -100s second acquisition times. The microfluidic geometry enables the variation of both flow type and magnitude, beyond traditional rheo- SANS setups, and is exceptionally well-suited for complex fluids due to the commensurability of relevant time and lengthscales. We demonstrate our approach by investigating concentrated surfactant solutions and microemulsions, which exhibit strong flow response and relaxation. Specifically, we have studied sodium dodecyl sulphate (SDS)/octanol/brine, cetyltrimethyl ammonium chloride (C_{16}TAC)/pentanol/water, microemulsion ($C_{10}E_4$ /decane/ D_2O), using selective deuterium labeling. We determine relevant lamellae spacing, orientation and order parameter as a function of flow type and rate. Our approach opens opportunities for investigating soft matter under flow and confinement using SANS, with industrial relevance including formulation engineering and oil recovery.

Interfacial rheology of model particles at liquid interfaces

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Particle-stabilized liquid-liquid composites, including Pickering-Ramsden (PR) emulsions and bijels, have received considerable attention in recent years. The reasons for this are twofold: (1) PR composites are model arrested systems and (2) they have significant potential for applications in foods, personal-care products and catalyst supports.

It has been demonstrated that the role of interfacial particles in stabilizing liquid-liquid composites can be quantified using interfacial rheology [1]. However, the full impact of interfacial rheology on the stability of PR composites remains far from fully understood. For example, equivalent particleladen interfaces in stable emulsions can appear solid-like under compression [2], but fluid-like under shear. This rich behaviour arises from a complex interplay between liquid-liquid tension and interfacial particles. What is currently lacking is a comprehensive investigation of the interfacial rheology of model colloids at liquid interfaces and how that relates to PR composite stability.

Here, we present our results on the interfacial rheology of model microspheres at liquid–air and liquid–liquid interfaces (Fig. 1(a)). We consider both sterically stabilized PMMA particles and chargestabilized silica particles, varying the wetting properties of the latter by wet-chemical functionalization. We confirm that particle wettability has a strong effect on interfacial rheology [3]. Moreover, we find that liquid interfaces laden with sterically stabilized rather than charge-stabilized particles have a markedly different mechanical response under both compression and shear (Fig.1(b)), which we attribute to the interfacial mobility of the individual particles.

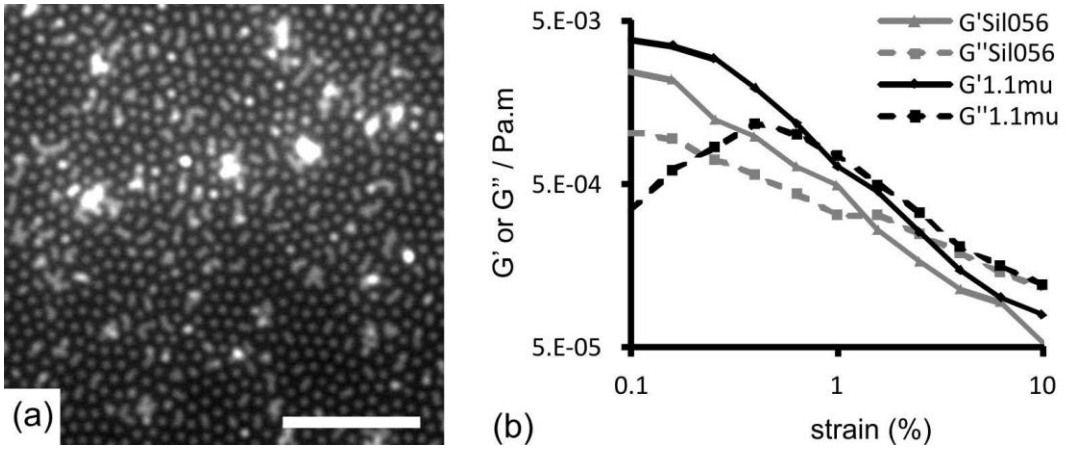

Figure 1: (a) fluorescence micrograph of 1.15 µm diameter particles at a water–oil interface. Colloidal particles are PMMA–PHSA i.e. poly(methyl methacrylate) sterically stabilized with poly(12-hydroxystearic acid); scale bar 25 µm. (b) Oscillatory strain sweeps at an angular frequency of 1 rad/s for 0.58 µm diameter silica spheres at a water–air interface ("Sil056") and 1.15 µm diameter PMMA–PHSA spheres at a water–oil interface ("1.1mu").

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(invited) Scaling laws of polymer membranes: from synthetics to nuclear envelopes and mechanotransduction

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Self-assembled membranes abound in biology, but lipids are not the entire story – protein polymer assemblies often add key physical properties to biological membranes. We have explored this with synthetic polymer membranes, called polymersomes, and also with the nuclear membrane or lamina that surrounds and protects the DNA in most eukaryotic cell types. Block copolymer amphiphiles of various molecular weights can generate vesicles, and we will review the broad variations of properties, including mechanical properties, as well as the segregation of mixed systems [1]. Our efforts with the nuclear lamina began with proteomics analyses of adult tissues [2] that reveal the nucleoskeletal protein lamin-A follows polymer physics scaling as a function of tissue elasticity, *E*, as do numerous collagens that directly determine *E*. Lamin-A confers a viscous stiffness to nuclei from high stress tissues where it predominates, whereas lamin-B's scale weakly with *E* and confer elasticity to nuclei. Differentiation of stem cells to fat or bone is respectively enhanced by low or high lamin-A levels, and nuclear entry of transcription factors prove to be lamin-A-regulated. Complementary insights are obtained for marrow cells for which nuclear deformability also regulates cell trafficking [3]. Tissue stiffness and stress thereby couple to lineage and lamins.

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Self-Assembly, Biomimetics and Pattern Formation

Orientational texture of lipid membrane domains

A Cohen Simonsen, J Dreier, J C Jeppesen, P L Hansen, J Brewer and J H Ipsen

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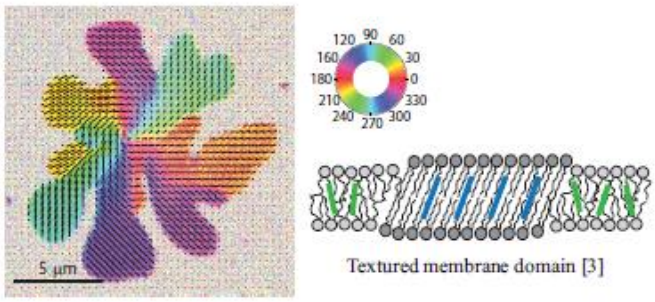
The principles underlying the in-plane organization of biomembranes remain incompletely understood more than 20 years after the proposition of the raft hypothesis[1]. Artificial model membranes with well-defined compositions have become some of the most useful systems for understanding domain formation in a controlled setting. Using advances in sample preparation and microscopy, new insights into the formation and structure of membrane domains are continuously being revealed.

We have focused attention on the gel phase, which can display a rich set of domain shapes and sizes as regulated by the growth kinetics and the spatial arrangement of nucleation points. Using polarized fluorescence imaging it was shown that gel domains in phospholipid membranes may contain long-ranged orientational texture patterns originating from the projection (the director) of the tilted acyl chains on the bilayer plane[2]. We visualize the texture using polarized 2-photon fluorescence microscopy and the Laurdan probe that aligns with the lipid acyl chains. An analysis of the signal variations with respect to polarization angle enables the lipid orientation to be resolved in single pixels. We have found that the texture of gel domains can exhibit topological defects including a vortex, pairs of half-integer vortices, and line defects[3]. The texture type is closely linked to the lipid composition as demonstrated by the occurrence of uniformly textured domains in some systems[4]. The texture patterns found in bilayer domains bear resemblance to smectic liquid crystal textures and textures in Langmuir monolayer domains and have also been associated with hexatic positional order of the lipids[5]. Texture represents a previously hidden level of complexity in the organization of bilayers, with potential unknown implications for the structuring of biomembranes. We provide an overview of orientational texture in a range of membrane systems and describe our efforts to understand and systematize defect types.



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Phase separation within hybrid polymer/lipid vesicles used as biomimetic membranes

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Hybrid vesicles resulting from the combined self-assembly of both amphiphilic copolymers and phospholipids may be viewed as an advanced vesicular structure compared to their liposome and polymersome forerunners, as the best from the two different systems can be integrated in a single hybrid vesicle and could be used in different fields such as: nano-reactors for enzymatic reactions, improved cell membrane mimics,[1], [2] etc… To afford such design, different parameters controlling both the self-assembly and membrane structure must be tuned. However, the exact mechanisms governing phase-separation of the membrane into domains analogous to lipid rafts in cells are not known so far. In this work, using different lipids and copolymers, we show that hydrophobic mismatch existing between polymer and lipid phase boundaries as well as the fluidity of the lipid phase are of prime importance on the membrane structuration, as schematically illustrated on Figure 1.

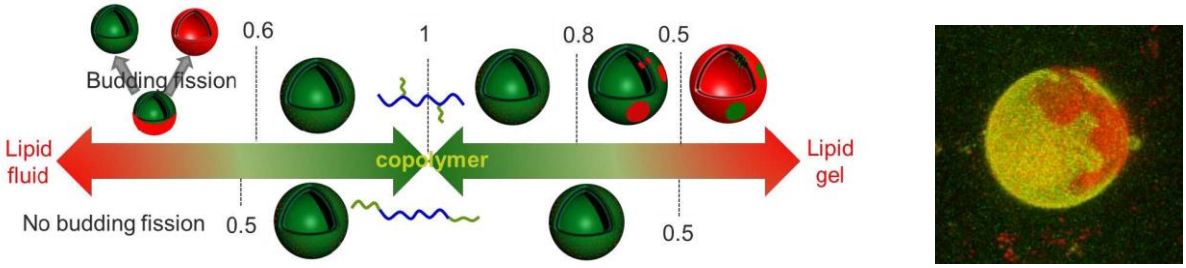

Figure 1: *Left:* Overview of the different hybrid vesicular structures that can be obtained according to the molar composition (polymer/lipid molar ratio) and thermodynamic phase of the phospholipid for a commercial graft copolymer $PDMS_{22}$-*g*-$(PEO_{12})_2$ and a triblock copolymer PEO_{17}-*b*-$PDMS_{68}$-*b*-PEO_{17} synthesized in the laboratory. *Right:* Confocal image

We have recently extended the study to small unilamellar Vesicles (SUV, D∼100nm) and obtained exciting preliminary results by SANS. Using deuteriated lipids and accurate D_2O/H_2O mixtures to match copolymer signal, we were able to detect only the lipid signal which can be fitted by a flat cylinder form factor giving a thickness $2H$=36 Å and a disc radius R_D=311 Å as shown on Figure 2. This strongly supports that phase separation occurs within the membrane, as observed for certain hybrid GUVs, and that the lipid phase probably adopts the shape of spherical cap(s) in the hybrid SUVs, which can be modeled with good approximation by flat disc shapes.

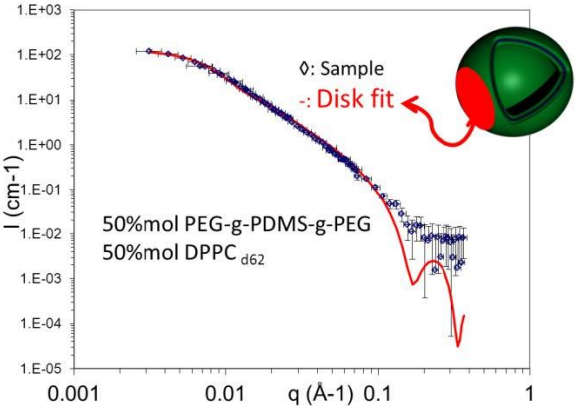

Figure 2: Intensity versus q fitted by cylinder form factor of 311Å radius and 36Å thickness (nano-disc)

Using lipids with different melting temperature and copolymers differing by their molecular weight, architecture (graft, di-block, triblock…) with similar hydrophobic and hydrophilic blokcs, we hope to establish a map of membrane structuration at micro and nanoscale and understand what are the molecular and macroscopic governing parameters of the phase separation. In that purpose, differential scanning calorimetry, Scattering techniques (light, Neutrons) as well as time resolved fluorescence spectroscopy (FRET) will be used for SUV in addition to Confocal microscopy for Giant vesicles. This study should clarify the elementary bricks necessary to modulate membrane properties of these new self assembled hybrid structures, in an optimized fashion regarding to different field of applications…

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Photo cross-linked and pH sensitive polymersomes - nanoreactor and membrane studies

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As part of the constant effort in science to mimic nature, amphiphilic block-copolymers were found to vesicles composed of a bilayer membrane. These so-called Polymersomes have proven to be suitable for synthetic biology such as drug delivery or nanoreactors. Compared to their biological counterpart, the liposomes, their membrane is considerably thicker and shows increased mechanical and chemical strength. This strength can yet be improved by introducing chemical bonds within the membrane, e.g. to crosslink it.[1] We combine membrane crosslinking on a photochemical basis with a pH sensitive polymer to give highly stable polymersomes with controlled permeability. Essentially, the transmembrane diffusion of these vesicles can be controlled by pH and the shear rate applied, which eventually lead us to the formation of a synthetic bionanoreactor.[2]

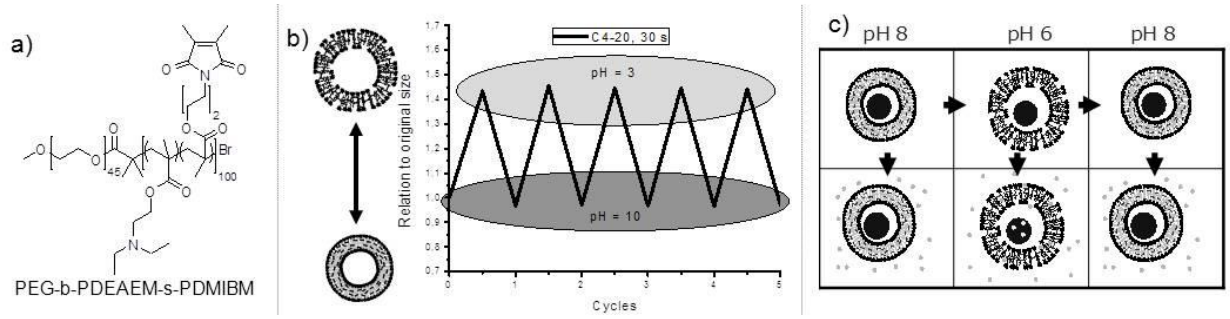

Figure 1. (a) PEG-b-PDEAEM-s-PDMIEM block-copolymer used to form polymersomes. (b) Reversible, pH cotrolled swelling behaviour. (c) Synthetic bionanoreactor allowing for reactions at an acidic state only.

Besides the possibility to make nanoreactors, this system also allows for a closer analysis of the membrane itself – as it is usually done for liposome membranes. Once spreaded on a Si wafer, we were able to cross-link the membrane once again and show significant changes in its mechanical properties upon cross-linking and a change in pH in terms of height and rigidity of the membrane. A combined analysis with AFM and confocal microscopy gave a deep insight into the mechanics of these vesicle-forming membranes.[3]

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Confined Fluids and Interfacial Phenomena

Crystal-liquid interfacial free energy via thermodynamic integration

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A novel thermodynamic integration (TI) scheme is presented to compute the crystal-liquid interfacial free energy (γ_{cl}) from molecular simulations. A key problem in previous thermodynamic-integration based approaches was the irreversibility and hysteresis inherent in the scheme due to the movement of the crystal-liquid interface. Here, by a clever approach of using extremely short-ranged walls to confine the liquid and crystal phases, whose actual contribution to the total interfacial free energy is negligible (<0.4%), we have made this irreversibility redundant.

Another feature of our scheme is the use of a frozen crystalline phase to act as a wall, instead of specially designed cleaving potentials (*J. Chem. Phys.*, 84, 5759 [1986]) or cleaving walls (*Phys. Rev. Lett.*, 85, 4751 [2000]). It is seen that this approach prevents the formation of metastable states during the transformation. Our technique is applied to compute (γ_{cl}) of systems interacting via Lennard-Jones and repulsive inverse-power ($\epsilon(\sigma/r)^{256}$) potentials. We obtain good agreement with previous works based on a cleaving-wall approach (*J. Phys. Chem. B*, 109, 17802, [2005]), non-equilibrium work methods (*J. Chem. Phys.,* 124, 034712 [2006]) and a metadynamics (*Phys. Rev. B.*, 81, 125416, [2010]) simulation.

Circularly confined quasi-hard-discs: the role of boundary adaptivity

I Williams[1,2,3], E C Oğuz[4], P Bartlett[3], H Löwen[4] and C P Royall[1,2,3]

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The behaviour of materials under spatial confinement is dramatically different from that in the bulk. The exact nature of behavioural modification in confined systems is strongly dependent on the boundary enclosing the system with soft walls inducing different phenomena than similar hard walls. In two dimensions, confinement within a hard circular boundary inhibits the hexagonal ordering observed in bulk systems at high density. Using colloidal experiments and Monte Carlo simulations, we investigate two model systems of quasi hard discs under circularly symmetric confinement.

The first system employs an adaptive circular boundary, defined experimentally using holographic optical tweezers [Fig. 1 (a)]. Deformation of this boundary enables mechanical pressure measurements to be made and allows hexagonal ordering in the confined system leading to the observation of a novel structural bistability between concentric particle layering and locally hexagonal configurations at high density [1]. Additionally, shearing the confined system drives this bistability resulting in the observation of a novel oscillatory state characterised by periodically self-similar structural organisation. Under varying conditions, both shear melted and rigid-body-like flow behaviour is observed.

The second system employs a circularly symmetric optical potential to confine particles without a physical boundary [Fig. 1 (b)]. We show that, in the absence of a curved wall, near perfect hexagonal ordering is possible. It is proposed that the degree to which hexagonal ordering is suppressed by a curved boundary is determined by the 'strictness' of that wall.

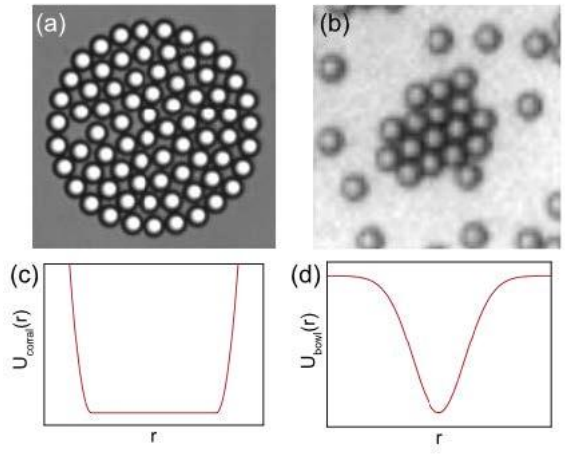

Fig. 1: (a,b) Micrographs illustrating experimental model systems. (c,d) Schematics of circularly symmetric potentials employed in experiments depicted in (a) and (b)

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Displacement mechanisms in micro-models from micro-fluidic experiments and pore scale lattice Boltzmann simulations

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For the purpose of CO2 storage in rock formations, it is important to enhance our fundamental understanding of the fluid displacement processes at the pore scale. This includes the injection of CO2 as a non-wetting fluid (drainage) followed by spontaneous imbibition of brine as a wetting fluid. These processes determine the initial and residual saturations of CO2 respectively. Obviously it is important to maximise the residual saturation for optimal CO2 storage. As it is difficult to visualise the displacement processes directly in real porous media, we have developed specific micro-fluidic models, with designs ranging from simple pore junctions to complex networks representing actual rock thin sections. First, we study drainage processes in single junctions and observe good agreement with Young-Laplace capillary filling rules, as shown by Lenormand et al. in their classic paper [1]. Then we investigate imbibition processes and confirm capillary filling rules are obeyed [2], in agreement with [1], provided that capillary pressure drop is sufficiently small. However, for larger capillary pressure drops, often associated with the process of spontaneous imbibition where the pressure drop cannot be controlled, we observe that the sequence of pore filling is determined by local pore geometry rather than the Young-Laplace law.

These new findings are confirmed by direct lattice-Boltzmann computer simulations in the same geometries. We are currently examining the consequences of these findings in complex etched micro-fluidic models. Our research suggests that imbibition displacement rules for CO2 sequestration may have to be revised. [3]

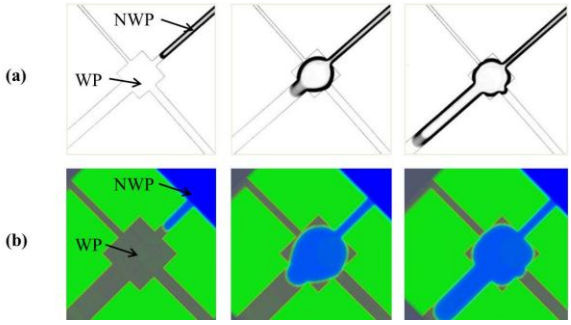

Figure 1: Dynamic drainage images: (a) experimental images of forced injection of non-wetting phase WP at 0.5ml/min (b) corresponding LBM simulations.

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(invited) Directed assembly in soft matter

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In directed assembly, applied fields are typically used to steer dispersed micro-particles into well-defined structures at given locations. Here, we exploit fields that arise spontaneously when particles are placed in contact with deformable matter. In one context, we use capillary interactions that occur between anisotropic microparticles at fluid interfaces. Energy stored in interfacial deformations and curvature fields can be used to direct particles to assemble with preferred orientations at well-defined locations. Recent results for anisotropic particles on curved interfaces will be discussed.

In another context, we exploit elastic energies and defect fields in confined liquid crystals. For example, by confining a nematic liquid crystal between surfaces with well-defined anchoring energies, the director and associated defect fields can be molded to store elastic energy. We explore this theme using topographically patterned solid surfaces to define defect fields in rings and other structures that steer particles into assemblies mimicking the defect texture, even for particles trapped at interfaces far from the disclination line that sources the migration. Related examples for particle migration in smectic films are discussed.

Surfactants, Foams and Vesicles

Unveiling the bifurcation diagram of pattern formation in surfactant monolayer transfer

M H Koepf[1] and U Thiele[2,3]

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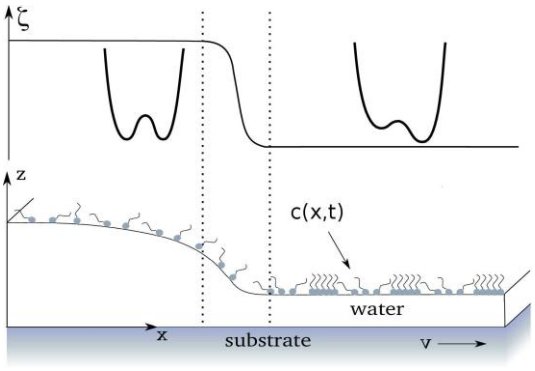
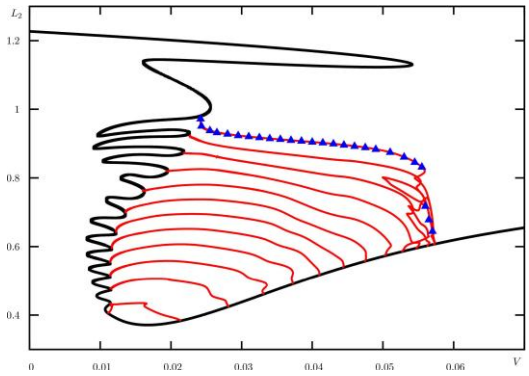
Spontaneous pattern formation in deposition processes at receding contact lines has become a versatile tool to coat substrates with well controlled micro- and nanostructures. As a paradigmatic example, the coating of substrates with periodically structured monolayers has in recent years been investigated by theoreticians [1,2] and experimentalists [3,4] alike. Here, we present recent progress [5], allowing for the first time to understand the intricate bifurcation diagram of the system that exhibits a snaking branch of stationary solutions. Each nose of the snake is connected to a branch of time periodic solutions. Using numerical continuation, we detect various local and global bifurcations and investigate how the solution structure depends on the system size. These results are of wide interest for the theoretical description of pattern formation in systems with nontrivial boundary conditions.





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Extreme deformation of giant unilamellar vesicles in a complex shear flow

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Giant unilamellar vesicles are useful model systems to study the dynamics of some cellular processes and transport phenomena, including viral infection, endocytosis, exocytosis, and cell fusion. In addition, vesicles find applications as vehicles for drug delivery and in the food industry. The response of vesicles to flow and deformation is central to these applications as it affects the non-Newtonian rheology of vesicle suspensions.

The dynamics of vesicles under small deformation in simple shear flow is relatively well understood. Complex behaviors are observed, such as tumbling, breathing, and tank-treading, depending on the viscosity contrast between interior and exterior fluid, excess area, membrane viscosity, and bending modulus [1-3]. On the contrary, phenomena upon extreme deformation are still poorly understood. These include shear-induced pore formation, membrane rupture, and vesicle lysis [4], which can be exploited in biomedical applications provided that they can be triggered in a controlled fashion.

We study the behavior of giant unilamellar vesicles in a complex microscale shear flow in an acoustofluidic setup. We explore the effect of lipid composition and resulting membrane properties (area expansion and bending modulus, membrane viscosity) on mechanisms of pore formation, rupture and lysis. Failure events are visualized using a fluorescence-based leakage assay.

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Foams stabilized by mixtures of nanoparticles and oppositely charged surfactants: Relationship between bubble shrinkage and foam coarsening

A Maestro[1,2], E Rio[1], W Drenckhan[1], D Langevin[1] and A Salonen[1]

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We believe that our work makes a significant contribution to understand how interfacial jamming and buckling can result in the stabilization of a foam. For our purpose, we use surfactant-decorated nanoparticles, which become irreversibly adsorbed at the gas/liquid interface. Compression of such a bubble leads first to an increase of the interfacial elasticity, before buckling of the surface is observed. In a collection of bubbles, a foam, gas transfer from smaller to larger bubbles also leads to a compression of the interfaces. If the particles are sufficiently highly packed they can become jammed, leading to solid-like behavior, and any further compression will result in the buckling of the interface, characterized by an undulating surface. Trough controlled experiments at multiple length-scales, starting with single interfaces and solitary bubbles, we are able to make qualitative predictions to the arrest of the coarsening through interfacial jamming and buckling.

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Optical Methods and Imaging

Exploring soft matter with X-ray scanning micro- and nano-diffraction techniques

E Di Cola

European Synchrotron Radiation Facility (ESRF), France

Detailed characterisation of hierarchical structures in soft matter and biological systems can be achieved by X-ray imaging methods using synchrotron radiation. Among the different approaches, X-ray scanning methods using micro- and nano-beams offer a powerful tool to locally map heterogeneous materials and obtain quantitative information with nanometre resolution. In the last years, strong effort has been put to improve the time and spatial resolution of the technique, to develop fast data acquisition systems, new strategies for sample manipulation, and radiation damage control. Therefore, scanning X-ray techniques are now routinely in use at synchrotron sources.

This contribution will demonstrate the unique opportunities offered by scanning small- and wide-angle X-ray techniques using micro- and nano-metric beams at beamline ID13 of the European Synchrotron Radiation Facility (ESRF). After a short overview of recent technical developments (sample positioning, new refractive focusing optics, increase in X-ray flux), the presentation will mainly focus on scientific examples from the field of biological hierarchical materials (such as wood and tissue) as well as of polymer composites. The quantitative interpretation of two-dimensional scattering and diffraction mappings of the samples will be demonstrated also in combination with complementary spectroscopic techniques. Adapted sample environments which allow in-situ mechanical deformation and thermal studies will be presented.

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Single cell monitoring of redox potential using Surface-enhanced Raman Spectroscopy

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School of Chemistry, University of Edinburgh, UK

Intracellular redox potential is involved in many cellular functions, such as the cell cycle, signalling and protein folding. It is tightly controlled, and its dysregulation is associated with several disease states, including cancer, inflammation and heart disease. We have created redox active probe molecules that change structure depending on their oxidation state, and developed a protocol for coating gold nanoshells with these probes. Surface-enhanced Raman spectroscopy (SERS) of the coated nanoshells allows spectral discrimination and quantification of the ratio of oxidised and reduced states, and thus calculation of the local redox potential.

The initial aim of this project was to optimise the protocols for rapidly and reproducibly acquiring SER spectra from our nanosensors in individual cells using a mapping technique (see figure). Current work is focused on methods for acquiring spectra from cells subjected to various oxygen concentrations and automating the data analysis of the SER spectra maps.

Further work will investigate how intracellular and extracellular redox potential are coupled and how redox potential changes at sub-physiological O_2 concentrations (in hypoxia). These new tools are likely to be useful for further developing our understanding of how altered redox potential may drive disease states.

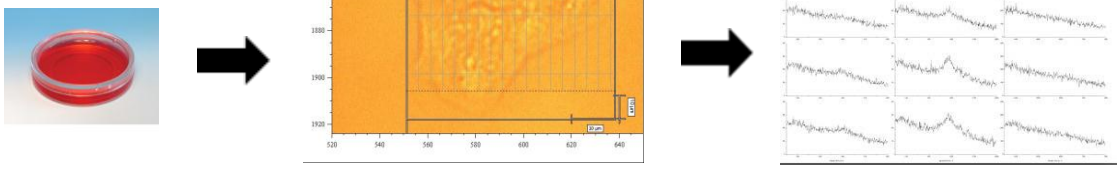

Plate cells in dish, add nanosensors

Select cell(s) to be imaged and perform map acquisition of spectra

An extract from a larger map, showing signals from one nanosensors inside a cell

Optical Coherence Tomography Velocimetry of complex fluids

A V Malm[1,2], S Jaradat[1,2], M Harvey[2], A W Harrison[1,2] and T A Waigh[1,2]

[1]Biological Physics Group, School of Physics and Astronomy, University of Manchester, UK, [2]Photon Science Institute, University of Manchester, UK

Optical Coherence Tomography (OCT) Velocimetry is a new technique for studying rheological systems that uses advances from medical imaging. It is a useful addition to the growing range of optical rheometry techniques [1].

Light is scattered off a sheared fluid and an interferometer with a low coherence infra-red light source allows Doppler signals to be measured for slices of fluid 9 microns thick, with a probe volume of 3.4 pico litres, allowing velocity profiles to be observed for opaque materials with sample thicknesses of several millimetres [2].

Studies of these velocity profiles allow a deeper level of understanding of complex flow phenomena than is possible with classical bulk rheology measurements. OCT Velocimetry is competitive with other velocimetry techniques in terms of spatial and temporal resolution as well as the range of materials it is able to probe [3].

OCT velocimetry has been demonstrated with a range of complex fluid samples including food stuffs (margarine and tomato sauce), polymeric samples, namely polyacrylamides (PAM) which display elastic turbulence related shear banding behaviour and wall slip depending on polymer concentration and molecular weight, Figure 1 [4], and hard sphere colloidal suspensions which display shear banding in dense suspensions.

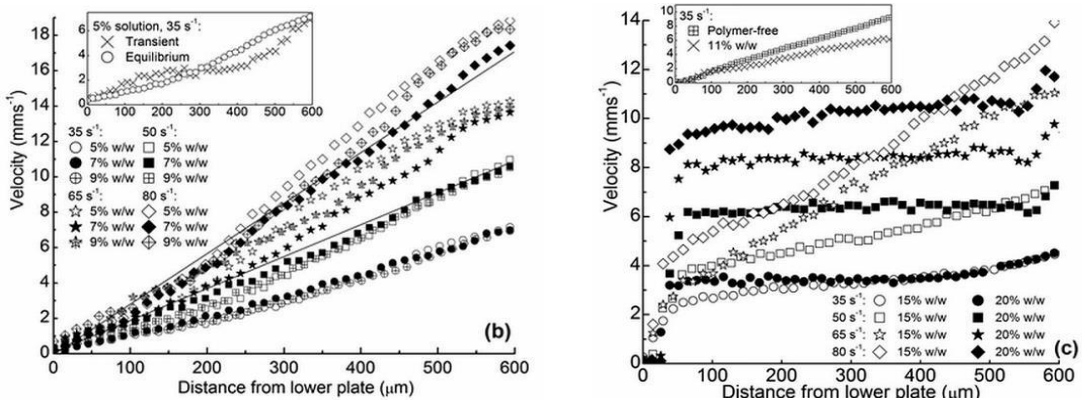

Figure 1: Left- Shear banding in PAM samples of 5% w/w concentration at a range of shear rates. Right- Wall slip in PAM samples of high concentrations (15% w/w and 20% w/w) at a range of shear rates.

We also present improvements to our original embodiment of the method, which uses modulation techniques and a Mach Zender interferometer in order to improve SNR and widen the measurable range of shear velocities.

The technique is also capable of providing quantitative measurement of velocity fluctuations of the flow, providing additional useful information on complex flow phenomena and the onset of turbulence.

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Wednesday 16 April

(invited) Self-assembly of patchy colloids

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We have developed new kinds of colloidal particles with either geometrical or chemical patches that give rise to directional interactions. These interactions allow colloids to interact with each other more like atoms, which in turn are used to build up structures that are not possible with isotropic interactions. These directional interactions are being developed to make self-replicating colloidal motifs and new colloidal crystals.

Colloids and Nanoparticles

Phase diagrams for magnetic nanofilaments

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Artificial magnetic filaments can be obtained by mutually linking magnetic colloids to form a chain. These magnetic chains represent the equivalent of magnetic polymers but at supra-molecular scale. In difference to one-dimensional chemical magnetic polymers which only manifest their magnetic properties at $T < 100K$, magnetic nanofilaments can retain their magnetism at room temperature and zero field.

The emerging interest in this relatively novel field is due to the fact that magnetic nanofilaments are very appealing from the technological point of view. They can be thought as improved substitutes of current ferrofluids, or as elements for magnetic memories, chemical and pressure nanosensors, nano-propellers, elements of nanopumps, non-permanent photonic crystals, or as generators of unique patterns able to provide watermarks to authenticate cards or other documents, to just mention a few possible applications.

In this contribution we will present the results of our ongoing numerical and theoretical studies[1–3] of flexible and semiflexible magnetic filaments for different physical environments. As an example of it, we will provide insight into the determination of the phase diagrams at zero field for magnetic filaments in which monomers exhibit short-range LJ attractive interactions (Stockmayer polymers, i.e. filaments in poor solvent conditions) in the limit of strong dilution, as well as filaments in good solvent conditions. The cases of magnetic chains in bulk (see figure 1) and near attractive surfaces will be thoroughly explored. Phase diagrams for those systems have been observed to exhibit a rich variety of new phases when compared with the phases for non-magnetic chains in similar environments.

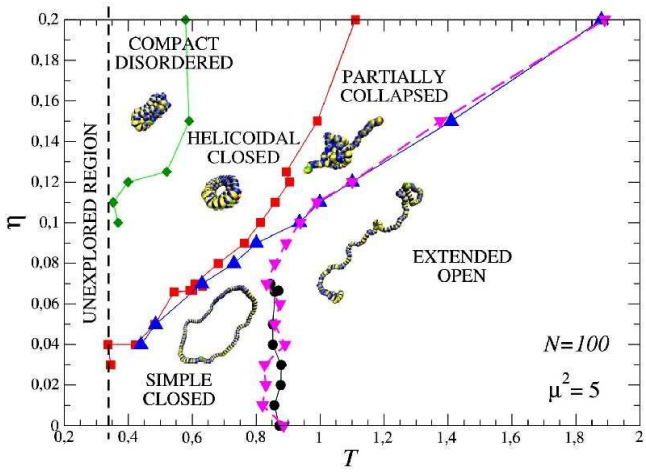

FIG. 1. A tentative phase diagram for magnetic filaments of length N=100, and a dipole moment per monomer of fixed strength $\mu^2 = 5$.

Acknowledgements: We thank the projects FISICOS (FIS2007-60327), GRID-CSIC and BwGrid founded by the Spanish MICNN and the ERDF, respectively.

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Colloidal aggregation and dynamics in anisotropic fluids

F Mondiot[1], R Botet[2], P Snabre[1], J-C Loudet[1] and O Mondain-Monval[1]

[1]University of Bordeaux, Center de Recherche Paul Pascal - CNRS, France, [2]University of Paris-Sud, Laboratoire de Physique des Solides, France

The formulation of colloidal particles/liquid crystals (LC) composites is a well-identified route towards the design of smart responsive materials with tunable optical or mechanical properties. However, the particles aggregate because they distort the intrinsic order of LC phases, which costs elastic energy. For micron-sized inclusions, the resulting elastic forces dominate the coarsening of the system. In this study, we find a new regime where elastic interactions no longer prevail when the particles are downsized to the nanometer scale. Instead, the system evolution is governed by an anisotropic Brownian diffusion coupled to attractive depletion interactions. This finding opens up new possibilities to better control the clustering of colloids in such media.

In our work, we present experiments and numerical simulations to investigate the collective behavior of sub-micrometer-sized particles immersed in a nematic micellar solution. We use latex spheres with diameters ranging from 190 nm to 780 nm and study their aggregation properties due to the interplay of the various colloidal forces at work in the system. We found that the morphology of aggregates strongly depends on the particle size with an evidence for two distinct regimes: the biggest inclusions clump together within minutes into either compact clusters or “V-like” structures that are completely consistent with attractive elastic interactions. On the contrary, the smallest particles form chains elongated along the nematic axis, within comparable time scales. In this regime, Monte Carlo simulations, based on a modified diffusion-limited cluster aggregation model, strongly suggest that the anisotropic rotational brownian motion of the clusters combined with short-range depletion interactions dominate the system coarsening; elastic interactions no longer prevail. The simulations reproduce the sharp transition between the two regimes upon increasing the particle size. We provide reasonable estimates to interpret our data and propose a likely scenario for colloidal aggregation. These results emphasize the growing importance of the diffusion of species at sub-optical-wavelength scales and raise a number of fundamental issues.

The effects of polydispersity and metastability on colloidal crystallization

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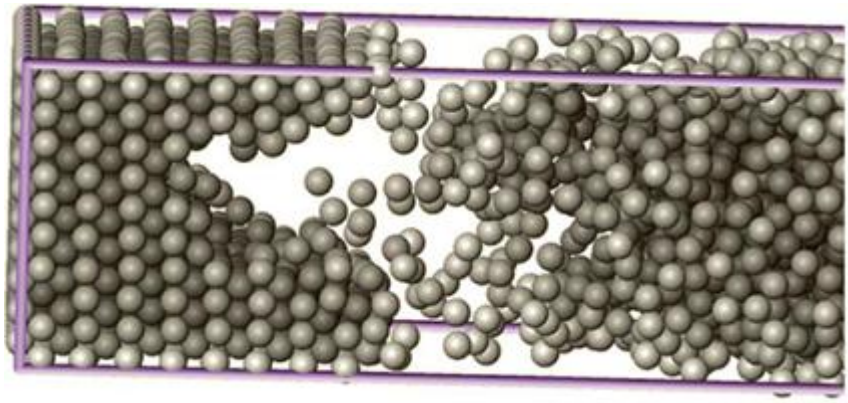
We have performed large-scale simulations of crystal growth in a system of slightly size-polydisperse particles, with important implications for the interpretation of any experiments involving metastability. Our system parameters are such that, in the vicinity of a metastable gas-liquid phase transition, a macroscopic layer of the colloidal-gas phase coats the crystal as it grows (see figure below), consistent with experiments and theoretical free energy considerations.

Crucially, the effect of this metastability on the crystal growth rate depends qualitatively on whether the system is polydisperse. We find a reduction in polydispersity and qualitatively different local size ordering in the crystal relative to the fluid, and propose that the particle-sorting required for crystallization is dynamically facilitated by the gas layer. Our results show that polydispersity and metastability, both ubiquitous in soft matter, must be considered in tandem if their dynamical effects are to be understood [1].



[1] The effects of polydispersity and metastability on colloidal crystallization, J J Williamson and R M L Evans, Soft Matter 9, 3600 (2013)

Self-Assembly

Epitaxy and polymorph selection in heterogeneous crystal nucleation

J P Mithen and R P Sear

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Crystallisation and its initial stage of nucleation are of widespread interest in many areas of soft matter physics [1]. Here we investigate two generic phenomena that are important for everyone who needs to understand crystallisation—epitaxy and polymorph selection. We use computer simulations in order to access the dynamics of crystallisation at the molecular scale, something that is difficult to do in experiments.

Epitaxy occurs when a crystal nucleating on a surface always forms with a particular fixed orientation to the surface lattice. To investigate epitaxy, we consider nucleation on a crystalline surface of a different substance (see Figure 1). Sixty years ago, Turnbull and Vonnegut predicted that a crystalline surface is best at inducing nucleation of another crystal when there is a perfect match between the two bulk lattices. Our computer simulations show that this is not quite right. In fact, the crystal lattice of a finite nucleus is strained from that in the bulk, and nucleation is fastest when the surface matches this strained lattice [2, 3]. We show that epitaxy can be predicted from relatively simple energy calculations.

Most substances exhibit multiple crystal forms, a phenomenon known as polymorphism. Controlling which polymorph crystallises is often of crucial importance, especially in the pharmaceuticals industry [4]. We offer some insights into how and why different polymorphs form based on computer simulations of a simple model system (see Figure 2).

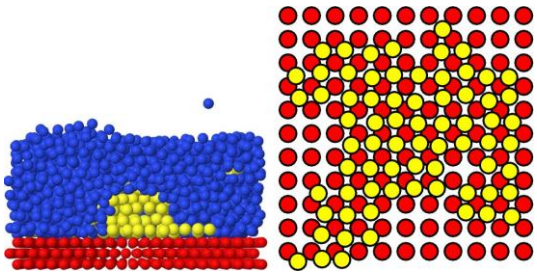

Figure 1: Nucleation on a crystalline surface. The surface is coloured red, the undercooled liquid blue, and the nucleus that has formed on the surface yellow. The left image is the simulation setup, the right image is a plan view with only the top layer of the surface and bottom layer of the nucleus shown. This is an example of epitaxy, where the orientation of the nucleus is fixed by the surface lattice.

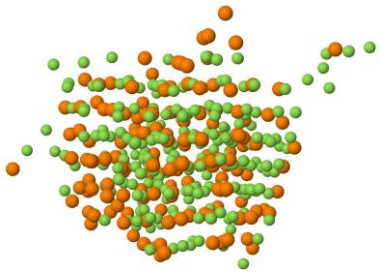

Figure 2: Competing polymorphs in crystal nucleation. The image shows a roughly 'critical' size nucleus, with some particles in a close-packed crystal environment (orange), and others in a body-centeredcubic environment (green). The image suggests that at the top of the nucleation barrier, the nucleus may not be one polymorph or the other, but a mixture.

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Simulation of polymer network formation: Phase behavior of aggregating chains

H Mortazavi and C Storm

Theory of Polymers and Soft Matter, Department of Applied Physics, Eindhoven University of Technology, The Netherlands

Filamentous biological materials display highly nonstandard mechanical response, among which a strong tendency to stiffen with increasing strain. This behavior is, in large part, determined by the stiffness of the constituent fibers and the degree of crosslinking among them. To replicate some of the properties of biological materials in a synthetic, self assembling system we study, experimentally and theoretically, the phase behavior of long, repeating copolymer motifs which alternate strongly hydrophobic bis-urea core blocks with long PEG spacers whose length may be varied. By tuning the relative importance of spacer entropy and core attractive energy, these molecules may either collapse, behave as random coils, or form an intermediate, network-like aggregate which shares important morphological characteristics with filamentous bionetworks. We present results from molecular dynamics studies of the phase behavior, and compare to the experimental findings.

Dynamic renormalisation group theory reveals sequential mechanism of oligomer generation in protein aggregation

T C T Michaels, P Arosio and T P J Knowles

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A key question in modern biochemistry and molecular biology is to determine the molecular pathways that control the overall kinetics of complex biochemical processes. Questions about mechanisms are usually difficult to answer using experimental techniques only, which can give clues, but rarely produce alone conclusive evidence for a given mechanism in systems characterised by the complexity of many biochemical processes. This limitation makes theoretical modelling an important tool as a complement to the experimental techniques.

An important class of biochemical processes, which are increasingly linked with biological function and disfunction, is the self-assembly of filamentous structures from soluble proteins. To date, only solutions to particular cases or solutions to the equations describing average quantities such as filament mass have been derived, which have identified monomer dependent secondary nucleation as the dominant mechanism in the aberrant self-assembly of soluble proteins into filaments[1]. A detailed knowledge of the sequential mechanisms behind the process of secondary nucleation, however, has been challenging to access, yet it is crucial for improving our understanding of the formation of low molecular weight oligomeric species, which appear likely to be the most toxic species.

We used the theoretical framework provided by the time dependent real-space renormalisation group (RG)[2] to connect the macroscopic features of fibril formation to the microscopic mechanisms of secondary nucleation through progressively more coarse-grained descriptions that yield simplified models to be compared with kinetic data. By analysing data from the polymerisation of islet amyloid polypeptides and the amyloid-β peptide Aβ42 into amyloid fibrils, we conclude that pre-critical nuclei stay attached to the aggregates during the process of secondary nucleation.

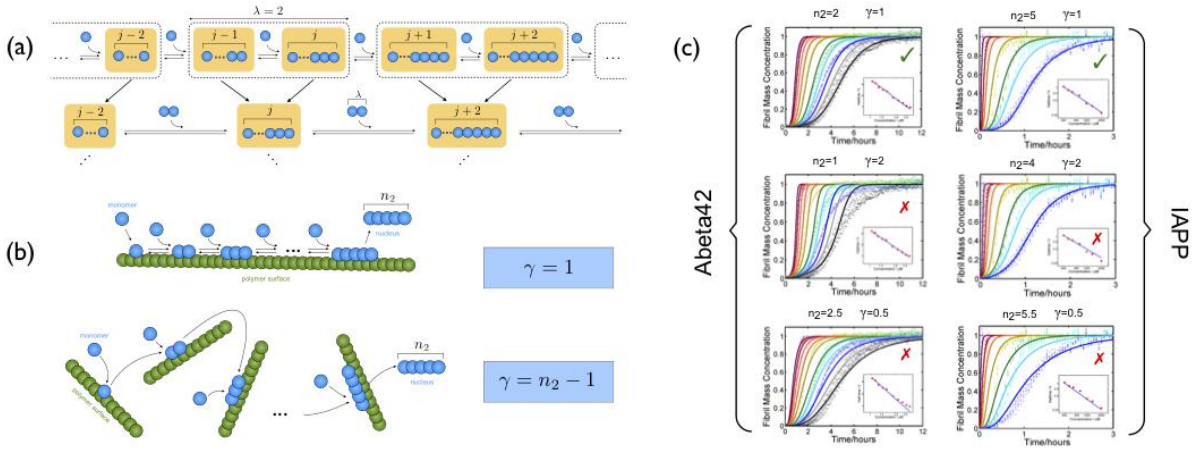

Figure 1 (a) Schematic representation of the RG transformation for nucleated polymerisation processes with representative decimation parameter $\lambda = 2$. (b) The RG analysis predicts that the various possible microscopic pictures of the secondary nucleation process are reflected by a different dependence of the secondary nucleation rate on the concentration of total fibril mass and soluble monomer. In particular, $r_2 = k_2 m(t)^{n2} M(t)^{\gamma}$, where $m(t)$ is the free monomer concentration and $M(t)$ is the polymer mass concentration. We display two limiting mechanisms of secondary nucleation. (c) RG theoretical analysis of the aggregation kinetics of Abeta42 and IAPP. The global fittings indicate clearly that the only combination of parameters compatible with the data corresponds to $\gamma = 1$ and $n_2 = 2, 5$, corresponding to the scenario, where new formed nuclei grow on the fibril surface before detaching.

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(invited) Single molecule studies of protein aggregation

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Small soluble protein aggregates are thought to play a key role in the initial development of neurodegenerative diseases, such as Alzheimer's and Parkinson's disease, but are difficult to study using conventional methods due to their low concentration and dynamic and heterogeneous nature. We have developed single molecule fluorescence based methods to detect and analyse the protein oligomers formed during an aggregation reaction, with time, and to study how these oligomers interact with the membrane of live neuronal cells. I will present recent work from our laboratory on beta amyloid, tau and alpha synuclein oligomers to show how such quantitative studies can provide new insights into both the aggregation pathway and also the molecular mechanism of cellular damage, allowing us to put forward a model for the disease onset.

Colloids and Nanoparticles

Ligand-mediated nanoparticle interactions at fluid-fluid interfaces

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Nanoparticle self-assembly at fluid-fluid interfaces is exploited in several emerging technologies including 2D functional nanomaterials with tunable properties [1]. In spite of their importance in determining the interfacial microstructure, our understanding of the pair interactions of nanoparticles at interfaces is still limited. Significant differences with nanoparticle interactions in the bulk arise due to the discontinuity in solvent properties at the interface. This discontinuity causes the grafted ligand layer on the particles to rearrange in asymmetric configurations that depend on ligand length and grafting density.

To gain insights in ligand-mediated nanoparticle interactions at interfaces, we measured the two-dimensional osmotic pressure (surface pressure) of a self-assembled nanoparticle monolayer in experiment [2]. The measurements were compared with the results of Brownian Dynamics simulations, which allow the calculation of the pressure due to entropy and interparticle interactions in the monolayer.

Computed pressure-density curves with a pair potential that accounts for ligand-mediated steric repulsion agree with experiment for a fitted value of the range of interaction that is in keeping with the contour length of the ligand used in experiment. This indirect measurement of the pair potential between ligand-capped nanoparticles at interfaces will be helpful in constraining future molecular dynamics simulations of nanoparticle systems.

This work provides insight into the pivotal role played by grafted ligands in the energetics and mechanics of nanoparticle-laden interfaces.

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Studying complex nanoparticle adsorption at liquid interfaces

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Trapping at the interface, combined with lateral mobility and the presence of specific interactions, makes self-assembly of colloidal particles at liquid-liquid interfaces (SALI) a process with huge potential for the creation of controlled structures, including novel ultrathin membranes and capsules.

It has been demonstrated that superparamagnetic iron oxide nanoparticles (NPs) stabilized by low molecular weight poly(ethylene glycol) (PEG) shells [1,2], adsorb and form saturated monolayers at water/oil interfaces [3,4]. Understanding the basics of this process is fundamental in directing the assembly of these NPs for applications. In particular, measuring the viscoelastic properties of the interfacial assemblies *in situ* and on the micro-scale is of upmost importance [5].

The effect of different PEG shells on the interfacial adsorption behaviour of the particles has been characterised using pendant drop tensiometry (PDT) at different concentrations. Particles with longer linear PEG chains show the highest surface activity and the fastest adsorption kinetics. Master curves have been created for the different particle types, demonstrating the concentration dependence of adsorption speed.

To further investigate the behaviour of the nanoparticles at the decane-water interface, the monolayer mechanical properties have been characterised via the tracking of passive probe particles of very different sizes. Micron-sized tracer particles, observed using fluorescence optical microscopy, show diffusive behaviour at the interface upon adsorption of the NPs. Fluorescence correlation spectroscopy (FCS), using quantum dots as tracers [6], was used to investigate the interface on the same length scale as the NPs. Surprisingly, these tracers also showed purely diffusive behaviour, with a progressive slowing down ascribed to NP adsorption. Using FCS, it was possible to follow the build-up of the NP monolayer with time, and to obtain master curves for the diffusion coefficient as a function of a concentration-dependent effective time, similar to the PDT master curves.

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Design of a fluorinated magneto-responsive material with tuneable ultrasound scattering properties

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Due to their numerous original properties, fluorinated materials are used in a wide variety of applications including coating agents for cooking devices or fabrics, ion exchange membranes or as biomaterials for cardiovascular implants. Owing to their very low solubility in water (less than 10 ppm) and, on the contrary, to their high

compressibility and ability to dissolve large quantity of gases (O_2, N_2, CO_2...), volatile fluorocarbons can be used for therapeutic applications in the inner components of ultrasound contrast agents (UCA), commonly referred as "microbubbles".

The UCA echogenicity relies on the impedance contrast between the tissues mainly made of water ($Z_{water} \approx 1.5\times10^6$ Rayl) and the materials to be injected, which is often a gas phase ($Z_{air} \approx$ 340 Rayl). However gas microbubbles also have a short lifetime due to their physicochemical instability in a fluid and tend to rapidly burst or to coalesce. One way to increase the lifetime of UCA in blood is to mix air with a perfluorocarbon gas that presents a very low solubility in the aqueous phase, thus acting as "osmotic agent" to slow down the Ostwald ripening process. Several routes were developed to obtain longer-lasting UCA, on the one hand by coating the bubbles with a stabilising shell of lipids or polymers [1,2], on the other hand by adding to air or nitrogen a partial pressure of a fluorinated gas, in that case wrapped by a shell of either hydrogenated [3] or F-alkylated double-tailed phospholipids[4]. Volatile fluoroalkanes incorporated in microbubbles are octafluoropropane [5], decafluorobutane, tetradecafluorohexane (commercialised as the Fluorinert™ FC-72 reference) [3,4], or perfluorooctylbromide (PFOBr) [2]. Recently, several teams reported the decoration of the surface of microbubbles with iron oxide nanoparticles, both for pure air [6] and for mixed air/fluorocarbon gas bubbles [5,7]. The idea was to be able to guide such magnetic microbubbles against the strong flow-rate of blood circulation by the use of a magnetic field gradient.

Thus, the US imaging community is still in search for alternatives to gas bubbles, which present a high echogenicity but poor long term stability. We propose here a new type of materials made of fluorinated ferrofluid oil droplets exhibiting both a large sound-speed contrast (1/3) with aqueous solution (500 $m\cdot s^{-1}$/1500 $m\cdot s^{-1}$) and sensitivity to an external magnetic fluid. The obtained objects are not only magnetically guidable but also present the originality to exhibit strong Mie resonances at specific frequencies [8], that vary depending on the intensity and the orientation of the external magnetic field with respect to the wave propagation vector [9]. When dispersed in a yield-stress hydrogel, these droplets exhibit outstanding magnetic-responsive attenuation properties. First, we will describe the process that was used to obtain the magnetic nanoparticles dispersed in the fluorinated oil. Then, we present the fabrication of the monodisperse emulsions in a yield-stress fluid and their acoustic characterisation. These results also pave the way to the realization of tuneable acoustic metamaterials [10]

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Liquid Crystals

On phase behaviour and dynamical signatures of charged platelet suspensions

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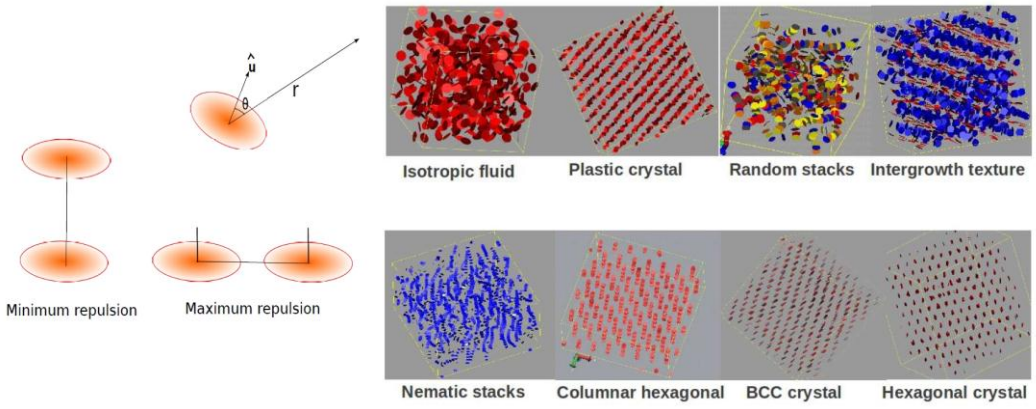
[1]LPTMS, CNRS and University of Paris-Sud, France, [2]LIPhy, UMR CNRS 5588, University of Joseph-Fourier, France, [3]University of Paris-Sud, Laboratoire de Physique Theórique, France, [4]Laboratoire de Physique des Solides, France, [5]Laboratoire PECSA,UMR 7195, Université Pierre et Marie Curie Case Courrier 51, France

Charged platelet suspensions, such as swelling clays, disc-like mineral crystallites or exfoliated nanosheets are ubiquitous in nature. Their phase behaviours are nevertheless still poorly understood: while some clay suspensions form arrested states at low densities, others exhibit an equilibrium isotropic-nematic transition at moderate densities. In the absence of electrostatic interactions, hard platelets undergo an isotropic-nematic transition as a result of the competition between orientational and positional entropy as predicted by the pioneering work of Onsager [1]. The main question that arises is: how electrostatic interactions influence the isotropic-nematic transition and the organisation of charged platelets?

To address this key issue, we investigate the competition between anisotropic excluded-volume and repulsive electrostatic interactions in suspensions of charged colloidal discs, by means of Monte-Carlo simulations and characterization of the dynamics of the structures. We use a first principle derived orientation-dependent effective pair potential [2] to investigate the phase behavior. The angular dependence of effective pair potential has a peculiar form that makes an asymmetry between two states of parallel disks in co-planar and stacked configurations (see figure, left part).



Exploring the phase behaviour as a function of platelets density and ionic strength, we find a rich a rich phase diagram (see figure, right part) that consists of various crystalline and liquidcrystalline structures. We show that the original intrinsic anisotropy of the electrostatic potential between charged platelets not only rationalizes generic features of the complex phase diagram of charged colloidal platelets such as Gibbsite and Beidellite clays, but also predicts the existence of novel structure of *intergrowth texture* that is composed of disks arranged in alternating nematic (red colour) and antinematic (blue colour) layers. Furthermore, studying the dynamics as a function of density, we provide a strong evidence of slowing-down of dynamics in the orientationally disordered states of charged platelets. This points to the potential formation of arrested states in some regions of phase diagram.

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Knotted defects in nematic liquid crystals

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We present a theoretical and computational investigation into the topological properties of knotted and linked line defects in nematics. We classify the number of topologically distinct field configurations one can associate to a given link, finding it equal to a well-known invariant - the determinant of the knot or link. Using the Pontryagin-Thom construction these distinct textures are understood in terms of Skyrmion tubes entangling the knot. We show the existence of metastable states containing such knotted and linked defects in cholesterics by numerical relaxation of the Landau-de Gennes free energy, finding knots whose size is comparable to the pitch length. We also present a set of robust topological rules for the resolution of disclination crossings based on the preservation of an induced orientation on defect lines.

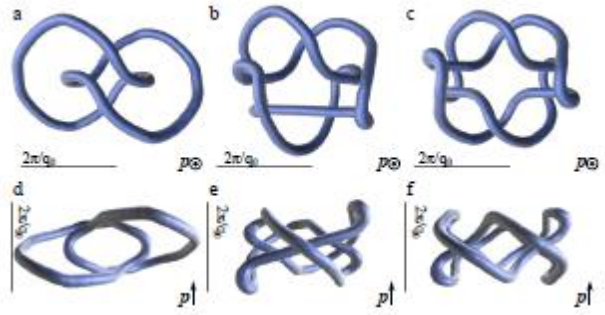

Figure 1: Images of stable knotted line defects in a cholesteric, found by numerical relaxation of the Landau-de Gennes free energy. Black lines indicate one pitch length. a, b & c are views along the pitch axis of a Hopf link, trefoil knot and Solomon's knot; d, e & f are views perpendicular to the pitch axis of the same knots.

Double twist liquid crystal model of collagen structure

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Dalhousie University, Canada

Collagen is the main component of connective tissue and the most abundant protein in mammals. The structure of collagen is hierarchical, with the triple-helical molecules organizing into fibrils, and fibrils contained in higher-order arrangements. A fibril may be considered as a liquid crystal of individual triple helices. Their chiral molecular structure can lead to a macroscopic helical arrangement known as the cholesteric phase, which has been observed in fragments of collagen fibrils. The cholesteric orientation can vary with radial distance in the fibril, this is known as a “double twist”. We numerically minimize the mean-field Frank free energy in the bulk to solve for the liquid crystal orientation as a function of radial distance, $\psi(r)$. By also considering surface terms, we find the optimal fibril radius R and molecule orientation on the fibril surface $\psi(R)$. We find that $K_3/K_2>>1$, where the twist modulus is much larger than the bend modulus, leads to a metastable minimum that recovers experimental measurements for R and $\psi(R)$ of collagen fibrils.

Poster Abstracts

Poster Session A

Biological systems

P.01 Mechanotransduction of deformable nano-structured elastic membrane surfaces on proliferation of osteoblast cells

G K Toworfe[1,3], R J Composto[2] and P Ducheyne[3]

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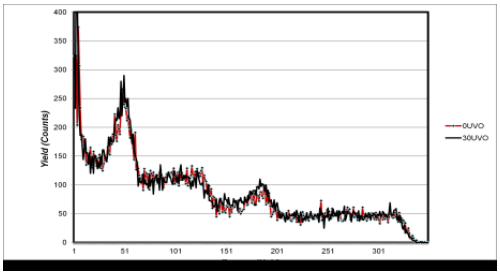
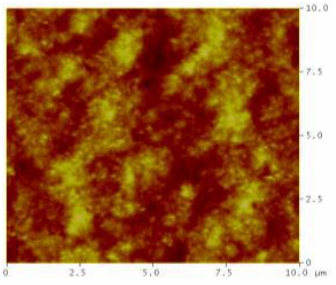
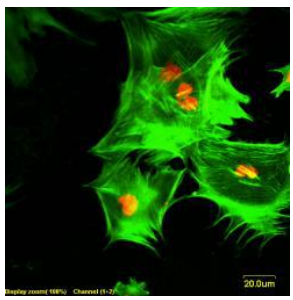
Bioactive substrates are capable of enhancing proliferation of osteoblast cells, since these cells transduce changes in the mechanical environment. This study investigates the effect of mechano-transduction through substrate characteristization on proliferation of osteoblasts-like (MC3T3-E1) cells. It is a fundamental study on the effect of mechanotransduction in bone cells through functionalised silastic bioactive nano-substrates. Strains occur in bone cells as a result of mechano-stimulus under physiological conditions [1] and the strain rate correlate with bone formation [2], since the mechanical forces are transmitted to cells through the ECM [3, 4] which results in immediate early gene expression and proliferation of MC3T3-E1 osteoblasts cells. Osteoblast cells were anchored to a chemically functionalized substrate to ascertain whether application of equibiaxial mechano-stimulus could change the cytoskeletal architecture of the cells. The membrane was functionalized, characterized using CA goniometry, RBS (fig. a) and AFM (fig. b). MC3T3-E1 cells were seeded onto the nano-scale biomimetic surface and subjected to mechanical deformation, after which cellular functions were evaluated, by CM, to determine changes in the cytoskeletal organization of the adherent cells. Application of biophysical forces to biological systems, according to Frost mechanostatic theory, translates into cellular responses, under physiological conditions; since cellular organisms tend to adapt to their mechanical environment. There were noticeable changes in the cytoskeletal architecture of MC3T3-E1 cells (fig. c) after subjecting them to the dynamic equibiaxial strains, with minimum cell damage, indicating that functionalised nano-surfaces transduced mechanical stimuli onto osteoblast-like cells. We engineered a system which mechanically transduces strains in nano-structured surfaces to enhance cytoskeletal architecture of osteoblast-like bone cells.



a) RBS data showing surface profile of membranes



b) AFM scans of radiated surfaces



c) CM-mechanotransduced MC3T3-E1 cells

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P.02 Streaming potential in human dentin

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Streaming potentials have been observed in wet bone and tendon [1-4]. Considering the compositions and microstructure of dentin have much in common with those of bone, it is of interest to investigate whether similar effects occur in dentin. The objective of this study is to reveal the streaming potential in human dentin and the related influencing factors.

Fresh human third molars without visible evidence of caries were used in this investigation. Flaky specimens, 4 mm (L) × 4 mm (W) × 0.8 mm (T), were prepared with two surfaces parallel to the occlusal surface and the others generally along tubules. A cell was designed and manufactured for facilitating the measurement of steaming potential in human dentin under a simulated physiological condition. A system including the cell, a mechanical testing machine, a scanner and a personal computer was established for cyclic loading and data acquisition. The streaming potential of the dentin specimens was evaluated under the loading frequency ranging from 0.05 to 0.2 Hz. Subsequently, a hole of 0.5 mm in diameter was drilled in each dentin specimen for simulating the effect of deep caries on the streaming potential in dentin, the streaming potential of these dentin specimens were reexamined.

The canaliculus system of solid is attributed to its streaming potential properties. Dentin is a biological composite formed by 50 vol.% mineral in the form of carbonated apatite, 30 vol.% organic component (mostly collagen) and 20 vol.% fluid, and has a distinct microstructure characterized by tubules that are the path of the odontoblasts during tooth formation. The tissue fluid in the dentin tubules could be regarded as electrolyte. Our investigation revealed the streaming potential in human dentin under testing condition (Tab. 1). The value of streaming potential increased with the increase of the frequency of cyclic loading (Fig. 1). The phenomenon may result from the increasing difference of pressure between the opposite surfaces of the dentin specimen upon the increase of velocity of the fluid through tubules as a result of increasing loading frequency. Introducing small hole into dentin specimen resulted in the decrease of peak streaming potential (Fig. 2). It was inferred from this experiment result that deep caries on decayed tooth had certain influence to streaming potential in dentin, with the peak value getting lower. However, the influence to the tooth under the physiological condition was not so obvious and still needed further research.

Table 1. Peak voltage (mV) of the streaming potential of dentin specimens

Frequency* (Hz)	Specimen#	
	Intact	Drilled
0.2	0.71 (0.06)	0.45 (0.08)
0.1	0.53 (0.03)	0.31 (0.06)
0.05	0.28 (0.05)	0.26 (0.04)

*P=0.003, #P=0.000

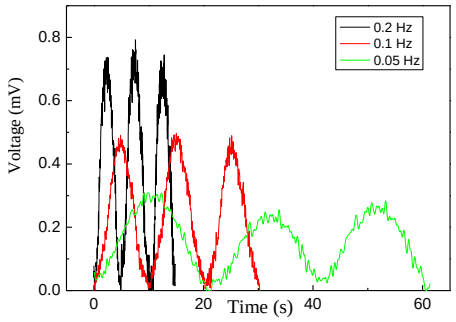

Fig 1. Streaming potential of dentin at the loading frequency of 0.2 Hz, 0.1 Hz and 0.05 Hz.

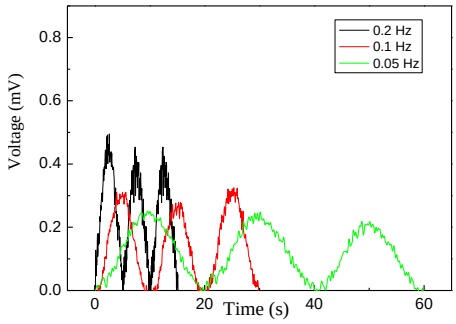

Fig 2. Streaming potential of drilled dentin at the loading frequency of 0.2 Hz, 0.1 Hz and 0.05 Hz.

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P.03 Structure and evolution of high-density protein systems

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This project aims to examine how whey proteins typically behave at the sub- molecular level under highly concentrated conditions where competition exists between the molecules for hydration-water. Freeze-dried bovine-derived beta-lactoglobulin (BLG, type-A) whey protein powder is dissolved at varying protein solution concentrations in two different aqueous buffer systems (0.2M Na_2HPO_4 and 0.1M Citric Acid, and Phosphate buffer). These protein solutions are buffered at pHs above and below the isoelectric point pI (pH$\sim$ 5.1). Infrared (ATR FTIR) and circular dichorism (CD) spectroscopic techniques are used to study the micro-structural arrangements of the protein when solutions of proteins are condensed towards the intended levels for high-protein foods. Changes in the protein secondary structure with respect to increased concentration and the possible reversibility of any molecular structural change via dilution with buffer was examined. ATR FTIR found significant secondary structure change occurring between 10mg/ml and 50mg/ml protein concentration with very little change occurring for concentrations

higher than 50mg/ml. This may be explained by the structure evolving from a less dense to a denser more compact inter-molecular β–sheet formation. Between 10mg/ml and 50mg/ml there was noticeable loss in α –helix structure signal and a simultaneous gain in random coil signal which may be interrelated (i.e. one structure replacing the other with increasing concentration). This is the concentration range over which the vast majority of secondary structure change seems to happen with little change occurring beyond 50mg/ml. These changes were verified by the CD method with the additional suggestion of aggregates occurring with increasing concentration.

P.04 Dynamics of filopodium-like protrusion and endothelial cellular motility on 1-D extracellular matrix fibrils

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Endothelial filopodia play key roles in guiding the tubular sprouting during angiogenesis. However, their dynamic morphological characteristics, with the associated implications in cell motility, have been subjected to limited investigations. In the present work, the interaction between endothelial cells and extracellular matrix fibrils was recapitulated *in vitro*, where a specific focus was paid to derive the key morphological parameters to define the dynamics of filopodium-like protrusion during cell motility. Based on 1-D gelatin fibrils patterned by near-field electrospinning (NFES), we study the response of endothelial cells (EA.hy926) under normal culture or ROCK inhibition. It is shown that the behavior of temporal protrusion length *vs.* cell motility can be divided into distinct modes. Persistent migration was found to be one of the modes which permitted cell displacement for over 300μm at a speed of 1μm/min. ROCK inhibition resulted in abnormally long protrusions, and diminished the persistent migration, but dramatically increased the speeds of protrusion extension and retraction. Finally, we also report the breakage of protrusion during cell motility, and examine its phenotypic behaviors.

P.05 Modelling of the Nuclear Pore Complex

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The Nuclear Pore Complex (NPC) forms a selective gate for all transport between the nucleus and the cytoplasm in the living cell. Its selectivity for larger macromolecules relies on changes in a permability barrier that is formed by unstructured proteins, induced by interactions of these proteins with so-called importins and exportins. The exact mechanism by which this works is unknown. We have modelled the NPC as a polymer-coated cylindrical pore via classical Density Functional Theory (DFT) and Monte Carlo (MC) approaches, to show that - for physiologically relevant parameters - the pore can act as a bi-stable switch, in which small changes in polymer-polymer interaction causes the system to switch between a closed, centrally condensed state and an open state in which the polymers condense at the pore wall. We have then extended this work to look at the effects of different macromolecules upon the conformation of the polymers in the pore. We will present direct comparisons of our results to experiments done on the NPC.

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P.06 Effect of solvent on the self-assembly of Dialanine and Diphenylalanine Peptides

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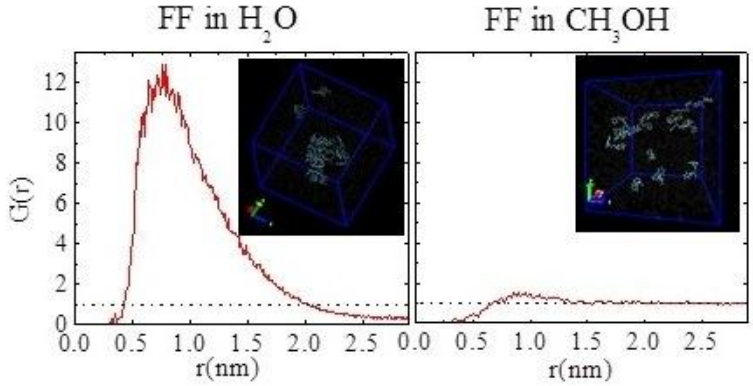
Diphenylalanine (FF) is a very common peptide with many potential applications, both biological and technological, due to a large number of different nanostructures which it attains. The current work concerns a detailed study of the self assembled structures of FF in two different solvents, an aqueous (H_2O) and an organic (CH_3OH) through simulations and experiments. Detailed atomistic Molecular Dynamics (MD) simulations of FF in both solvents have been performed, using an explicit solvent model. The self assembling propensity of FF in water is obvious while, in methanol a very weak self assembling propensity is observed. We studied and compared structural properties of FF in the two different solvents and a comparison with a system of dialanine (AA) in the corresponding solvents was also performed. In addition, temperature dependence studies were carried out. Finally, the simulation predictions were compared to new experimental data, which were produced in the framework of the present work. A very good qualitative agreement between simulation and experimental observations was found.



In the above figure the pair radial distribution function (rdf) calculated for the center of mass (cm) of peptides: (*left*) FF-FF in water and (*right*) FF-FF in methanol, at *T=300K* and *c=0.0385grFF/*(*cm*^{3}solvent) is presented. In the insets snapshots of FF in the corresponding solvents are shown.

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P.07 Double-belt a novel structure of membrane pore

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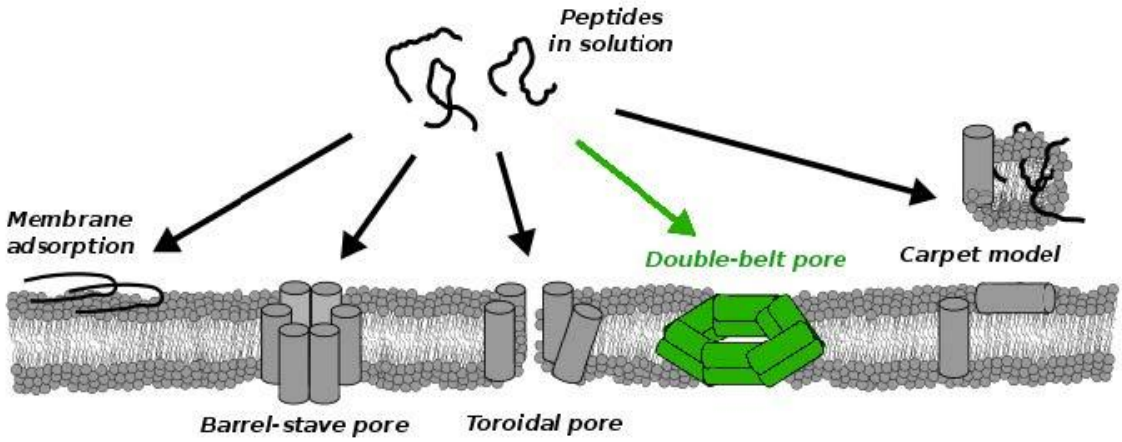
Amphiphilic proteins and peptides can induce formation of stable and metastable pores in phospholipid membranes, which has been associated with toxicity or antimicrobial activity. Using coarse-grained simulations we have studied peptide orientation within the pores and have found that peptides can be oriented perpendicular, parallel, or tilted with respect to the membrane plane. The orientation depends on the length of the peptide and its hydrophobicity distribution, which we rationalized in terms of the hydrophobic mismatch. Apart from well-known barrel-stave or toroidal pores our simulations suggest a novel 'double-belt' pore structure, where peptides within the membrane pore are oriented parallel to the membrane plane. This result was verified using more detailed

simulations with the MARTINI force field, where the double-belt structure was stable in micro-second time scale of our simulation.



P.08 Induced guidance of NIH 3T3 fibroblasts on Polydimethylsiloxane (PDMS) ridge-groove substrates: a time-lapse live-cell study

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Adherent mammalian cells and micro-organisms typically exhibit distinctive responses towards substrates with particular textures; the textures can be topographical, chemical, or both. Textured surfaces are readily observed to influence a cell's migration direction, alignment, adhesion, morphology, and even differentiation. Although the phenomenon has been extensively surveyed on different types of cells and on a variety of surface textures, the exact dynamical picture of how the cells are influenced by its underlying substrate has yet to be revealed. By creating thin film ridge-groove structures from polydimethylsiloxane (PDMS), we were able to probe, using live-cell methods, the dynamic interactions between cells and surface topographies at greater resolutions. Our investigations on NIH 3T3 murine fibroblasts revealed that the cellular protrusions lamellipodia and filopodia readily bend over the 90 degree angle at the ridge edge. Nevertheless, despite the versatility of these cellular protrusions, the 3T3s rarely trafficked from the ridge into the groove, or vice versa. In fact, if using the cell nucleus as the determinant in identifying ridge or groove cells, out of the 51 cases of 3T3s tracked over 10 hours on average, only 3 instances were observed where the cell trafficked across the ridge edge. Intuitively, this suggests possible contributions from the cell nucleus towards cell-topography interaction. Contemplating that nucleus' stiffness would potentially impose enough mechanical resistance when incident upon the edge, the nucleus stiffness of our 3T3s were modified using the histone deacetylases inhibitor, trichostatin A (TSA). It has been shown that this drug loosens the chromatin and subsequently induces a reduction in nuclear stiffness by as much as 60%. However, our results do not show an improved migration across the ridge edge, even with this much modulation in nucleus stiffness. Specifically, 37 3T3s incubated with TSA were tracked, but only one event showed the nucleus crossing the ridge edge. This result can, by no means, discount influences from nuclear stiffness though, but merely that a greater reduction in the nucleus' stiffness maybe required before the influence is revealed. There may also be possibilities of other determinants towards this topographical restriction. And to further complement our results we will also investigate into the contributions from cytoskeletal components; in particular the filamentous actin (F-actin). We plan to adopt live-cell time-lapse imaging of F-actin through the transfection of the Lifeact plasmid; this plasmid DNA, when expressed in the cell, produces green fluorescent protein (GFP) tagged markers that stain F-actins. The purpose of this endeavor is to identify any cytoplasmic actin structures that may be induced by the edge restrictions, which in turn restricts the cell nucleuses.

P.09 Influence of Ibupropfen on the structure of phospholipid layers

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Nonsteroidal anti-inflammatory drugs (NSAID) such as Ibuprofen have a wide range of medical applications, ranging from pain relieve over Alzheimer's [1] to cancer treatment [2]. However, some applications require long-term application, which can lead to gastrointenstinal complications and even fatal ulcers [3]. Neutron reflectometry and grazing incidence neutron scattering (GISANS) investigations of lipid films, which are excellent model systems for naturally occurring cell membranes, revealed a change in layer thickness upon the introduction of Ibuprofen[4]. This change in layer thickness can be attributed to a different apparent hydration of the film [5].

We investigated the influence of ibuprofen on phospholipid layers of L-α-phosphatidylcholine (SoyPC) between 0 and 33 wt% of ibuprofen. Our investigations have revealed that ibuprofen induces a two-step ordering in such films depending on the concentration. This ordering coincides with an initial increase and subsequent decrease in thickness, which can be attributed to a difference in the hydration of the layers (Fig. 1 a). Additionally, while there is no ordering for the pure SoyPC film, at 20 wt% ordering occurs. This ordering we identified as hexagonal with a superstructure. This superstructure vanishes at 25wt% of ibuprofen (Fig. 1 b) through d)), leaving a simple hexagonal structure.

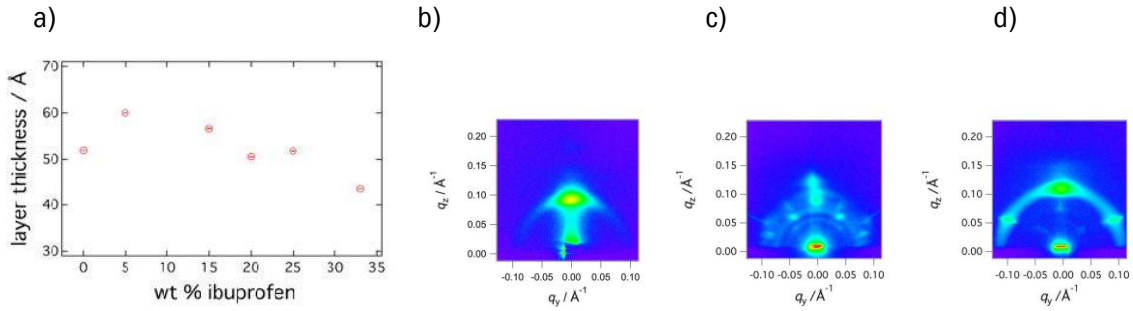

Fig.1. *a)thickness of layers in ibuprofen films at various ibuprofen concentrations,GISANS images at an incident angle of 0.2° for b) 0wt% ibuprofen, c) 20wt% ibuprofen and d) 25 wt% ibuprofen.*

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P.10 Study of cellular differentiation of embryonic carcinoma stem cells by AFM nanocytomechanics and Raman spectroscopy

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Studying the physics of biological systems is essential to deeply understand their behaviour. An in-depth investigation of the relationship between nanomechanical and biochemical signatures of biological systems is pivotal to improve our knowledge of the factors that influence their functions [1,2]. The biomechanical and biochemical markers of the undifferentiated stem cell status were obtained by combining Atomic Force Microscopy (AFM) nanoimaging and nanomechanics with Raman spectroscopy (RS). We used undifferentiated P19 embryonal

carcinoma cells, a well-established model system, and exposed them to uniform differentiation instructive factors, such as retinoic acid (RA) and dimethyl sulfoxide (DMSO), to induce differentiation into neural and cardiomyocyte cells without initial formation of embryonic bodies (EBs). The main difference between undifferentiated and differentiated P19 cells was found to be in their shapes. Neurons are the largest and thickest cells compared to cardiomyocyte and undifferentiated P19 cells as indicated by their surface area and apparent volume (Fig. 1). Also the organisation of the cytoskeleton (Fig. 2) showed substantial differences. While undifferentiated P19 cells presented thin actin filaments running from the nuclear region towards the edge of the cell, the differentiated cells showed either thick actin filaments running parallel (neurons) or woven actin filaments (cardiomyocytes). As a consequence, differentiated cells displayed a higher surface roughness than undifferentiated P19 cells. Cell elasticity was found to be one of the main nanomechanical markers. Undifferentiated p19 cells were found to be more elastically deformable than differentiated cells. Interestingly, the adhesion energy of P19 cells was higher than that of cardiomyocytes but lower than that of neurons, indicating a difference in the cellular membrane fluidity. RS indicated clear differences in the biochemical makeup of cellular differentiation status of P19 stem cells. Differentiated neurons and cardyomyocites showed a decrease in DNA content, and therefore proliferation and cell growth, than undifferentiated cells. Moreover, neurons were characterised by higher protein content than P19 cells, whereas cardyomyctes displayed a decrease in the protein contents. These results demonstrate the great potential of the AFM/Raman combination as a tool for the profiling of differentiated and undifferentiated cells.

Fig 1

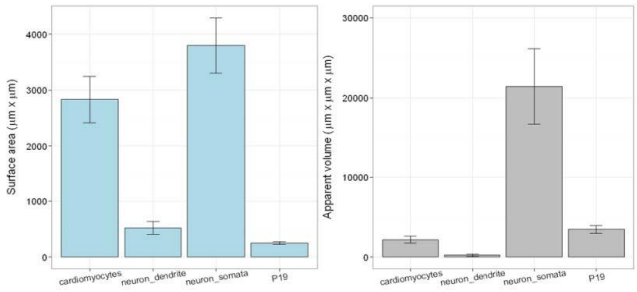
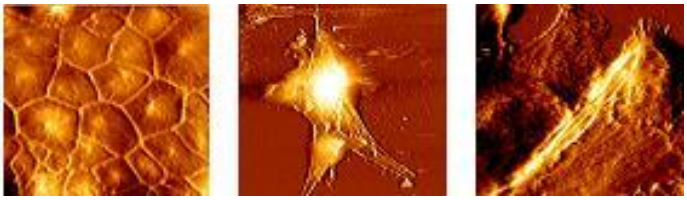


Fig 2



P19 **neurons** **cardiomyocytes**

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P.11 New insight into the structure and function of Hfq carboxyl terminus

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Accumulating evidence indicates that assemblies of essential components of RNA metabolism are localized on the cytoplasmic membrane of the bacterial cell, and that this cellular compartmentalization plays important roles to process RNAs. These assemblies include Hfq, the RNA chaperone protein, which is involved in the post-

transcriptional control of protein synthesis by virtue of its interactions with several small regulatory RNAs. Structurally, Hfq possesses two domains. The N-terminal domain folds as a five strongly bent β-sheets within individual protomers to assemble into a typical toroidal hexameric ring with a continuous β-sheet. The C-terminal flexible domain, which represents about one-third of the protein, seems intrinsically unstructured and most of 3D structures of Hfq lack C-terminal region. While the RNA binding core of Hfq lies within its Nterminal domain, the function of the flexible domain is controversial and remains largely unknown. We recently showed that this C-terminal region is responsible for the self-assembly of the protein into long fibers and that this property is associated with the ability of Hfq to localize within organized cellular structures in the vicinity of the membrane. Our progress toward studying the architecture of these ordered fibrillar ultrastructures formed by Hfq C-terminal domain will be presented during this meeting.

P.12 Single cell measurements of intracellular signaling, and motility, in activated macrophages

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Macrophages are cells of the vertebrate innate immune system. They are the only cells able to eat colloidal scale particles and bacteria. Macrophages move around the body to explore the environment and with their receptors they are able to detect the presence of pathogens. When this happens a complex network of signal pathways is triggered on. In this particular state the macrophage is "activated". The aim of our research is the characterization of the activation process in macrophages, via the investigation of both the NF-kB intracellular signaling pathway and the observation of motility and morphological cell phenotypes.

Regarding the intracellular signaling we propose a single cell approach to a better understanding of the TLR4 receptor and its role in the activation of the NF-kB pathway inside macrophage cells. We developed custom-build image segmentation software that enables the detection of NF-kB translocation within the cell. This method allows us to have quantitative direct measurements and to discriminate common trends and differences between different individual cells. On a bigger scale, from the point of view of cell motility, we investigate if the migratory behavior of macrophages changes depending on the different activation agents in order to fulfil specific biological needs. With this aim we conducted experiments to observe cells behaviors after stimulation from LPS (a molecule present on the outer membrane of gram-negative bacteria) and IFN-γ (used by macrophages for intercellular communication).

Colloids and nanoparticles

P.13 Restricted diffusion of small probe particles in a laponite dispersion

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Evanescent wave microscopy is used to study the dynamics of probe particles inside a laponite suspension, when the size of the latex probes is of the order of the diameter of the laponite disks. A correlation procedure is introduced that allows us to study quantitatively the diffusion of small probes.

For all studied sizes, the motion exhibits two modes: a fast relaxation mode and a slow relaxation mode. In the fast relaxation mode, the probes diffuse in a viscous medium, whose viscosity does not depend on the diameter of the probes and is slightly larger than the viscosity of water. Then, the diffusion of the particles is restricted over distances larger than their diameters, which increase when the particle diameter decreases.

In this regime, the probe particles experience the elasticity of the solution and the apparent elastic modulus increases when the diameter of the probe particle increases, whereas for large enough particles, the macroscopic

behavior is recovered, in which the diffusing particles experience a homogeneous medium, and the macroscopic elastic modulus is recovered.

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P.14 Dynamic properties of concentrated microgel suspensions and protein solutions

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Microgel suspensions and protein solutions exhibit interesting dynamical behavior, reflected in transport properties such as the generalized sedimentation and self-diffusion coefficients, and the viscosity. These properties are determined by the interplay of direct and hydrodynamic interactions. Using a simple spherical annulus model to account for solvent permeability, we have calculated analytically the hydrodynamic function of neutral microgel suspensions [1], in good agreement with experimental data [2]. We also present results for the self-diffusion coefficient and viscosity in comparison with simulations [3].

In addition, we use our analytic toolbox to study the effect of competing short-range attractive and longrange repulsive interactions on the dynamic clustering of globular protein solutions [4]. We study in particular diffusion properties, and the high-frequency viscosity.

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P.15 Detachment energies of spheroidal particles from liquid-liquid interfaces

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The energy required to detach a single particle from a liquid-liquid interface is an important parameter for designing certain soft materials: e.g. emulsions stabilised by colloidal particles [1, 2], colloidosomes designed for targeted drug delivery [3], and bio-sensors composed of magnetic particles at liquid-liquid interfaces. Calculating the detachment energy of spheroids necessitates the difficult measurement of particle-fluid surface tensions [4] -in contrast to spheres, where the contact-angle suffices. We develop a simplified detachment energy model for spheroids involving only the particle aspect-ratio and the height of the particle centre-of-mass above the liquid-liquid interface. By simulating the detachment of a single particle from a liquid-liquid interface using a

multicomponent lattice-Boltzmann model, we validate the model and provide further quantitative evidence for the use of lattice-Boltzmann methods in the simulation of particle-stabilised emulsions[5].

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P.16 Bicontinuous emulsions stabilized by nanoparticles

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Bicontinuous interfacially-jammed emulsion gels (bijels) are a relatively new class of versatile soft materials with a number of possible technological applications including tissue engineering, materials templating, fuel cells and microfluidics. They are produced by arresting the spinodal decomposition of a binary liquid mixture using neutrally-wetting colloidal particles which sequester to the liquid-liquid-interface, resulting in two tortuous interlocking channels (see Figure 1). Initially predicted by simulation in 2005[1] and subsequently realised experimentally in 2007[2], open questions regarding the formation of bijels and their long-term stability remain.

For various applications, smaller channels than the typical tens of microns (achieved using micron-sized particles) would be advantageous. Channel width L should scale as $\sim r/\varphi$, where r is the particle radius and φ the particle volume fraction[3]. Hence, nanoparticles could be used to achieve the reduction in pore size. However, simulations suggest that nanoparticle-stabilised bijels may not necessarily be stable at long timescales, since the particle attachment energy scales with r^2.

Here we show that by using nanoparticles we can reduce the channel width approximately fivefold at constant volume fraction. Stöber silica spheres are used to stabilise a bijel of the binary pair water and 2,6-lutidine, the structure of which appears stable over many weeks. Like the bijels made with micron sized particles, a ‘monogel’ is formed, so that the interfacial layer of nanoparticles remains intact after the remixing of the two liquids[4], which also allows post-processing into bicontinuous polymer-air composites[5].

Unlike their larger counterparts, the use of nanoparticles has mediated the use of much slower quench rates during the bijel preparation, from a minimum rate of 17°C/min down to as low as 1°C/min. Also, the prefactor in the scaling relationship $L \sim Cr/\varphi$ has increased, implying a lower interfacial uptake of particles. These results raise questions about the kinetics of binary liquid phase separation in the presence of colloidal particles of varying sizes.

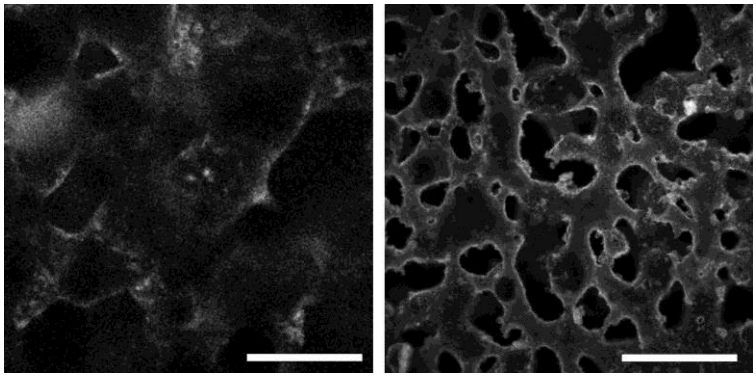

Figure 1. Confocal micrographs of bijels stabilized by (left) 250 nm and (right) 80 nm radius silica particles (white). Scale bar: 100 micron.

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P.17 Controlling ink properties to achieve a 'flatter' film profile for applications in P-OLED displays

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Polymer-Organic Light Emitting Diodes (P-OLEDs) are a technology where light is emitted as a function of the electrical operation. Unlike existing technologies, such as LCDs, they do not require a backlight with filters and they can be fabricated using a flexible, ultra-thin substrate rather than an inflexible layer of glass. For these reasons they have the potential for much larger viewing angles and for use in the next generation of flexible electronics applications, such as bendable mobile telephones [1] and curved television displays [2, 3].

P-OLED printed display panels (photos by Panasonic Corp.)

During the manufacturing process of P-OLED displays a solvent containing polymer ink, is dried. Depending on the processing conditions and ink properties a variety of different film profiles can be achieved. Typically the profile has some form of undulation, which results in a non-uniform emission profile and less than optimal efficiency and display lifetime. The aim of this project is to model the dynamics of the drying process in order to determine the final deposit shape. It is hoped that the model will enable prediction of conditions that will lead to 'flatter' profiles.

The model considers an axisymmetric, pinned droplet in which a 'coffee-ring' shape will develop due to an outward Capillary flow, as discovered by Deegan and co-workers [4]. This work has relevance for a plethora of other applications in which droplets containing a dispersed material are evaporated, such as blood disease diagnostics [5], fabrication of micro/nanowires [6] and distribution of pesticides on leaves. We have developed a code to predict the final film profile as a function of a single dimensionless group –the Capillary number, as well as the initial and maximal volume fractions of polymer. Using this we can explain the experimental evidence that was obtained with the aid of white light interferometry:

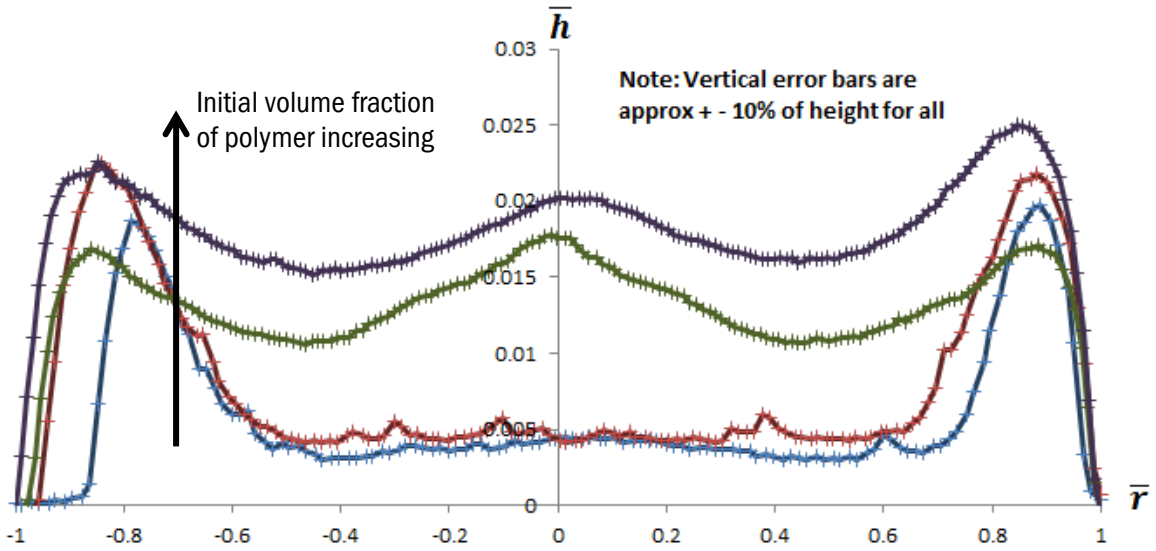

Figure: Dimensionless height against radius for droplets containing different initial polymer volume fractions

We will also present results for inks containing a mixture of solvents and discuss how the choice of ink formulation can help to achieve a flatter film profile.

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[4] Deegan et al., 1997, Nature, 389, pp. 827-829
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[6] Naqshbandi et al., 2012, Nature Communications 3:1188

P.18 Influence of magnetic field on the orientation of anisotropic magnetic particles at liquid interfaces

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We study theoretically the influence of an external magnetic field on the orientation of both ellipsoidal and cylindrical particles with a permanent magnetic dipole adsorbed at a liquid interface. The ability to control the orientation of such anisotropic magnetic particles allows us to manufacture novel materials with tunable mechanical, magnetic or photonic properties [1,2]. Specifically, using the finite element package Surface Evolver [3], we calculate the equilibrium meniscus shape around the anisotropic particles and equilibrium tilt angle when a magnetic field is applied perpendicular to the interface, inducing a magnetic torque on the anisotropic particles (see Fig.1). At zero field, the particles have a 'parallel' orientation ($\theta_t = 0$). However as we increase field strength, the equilibrium tilt angle θ_t increases, and at a critical magnetic field B_c and tilt angle θ_{tc}, the particles undergo a first order phase transition to the perpendicular orientation ($\theta_t = 90°$). We find that the critical field B_c increases with increasing aspect ratio of the anisotropic particles but decreases with increasing contact angle away from 90°. These results are in qualitative but not quantitative agreement with the simplified theory proposed by Bresme and

Faraudo [1] which assumes that the liquid interface is always flat. Our study demonstrates the importance of explicitly accounting for the deformation of the liquid meniscus for quantitative calculations of the orientation of magnetic anisotropic particles in an external field.

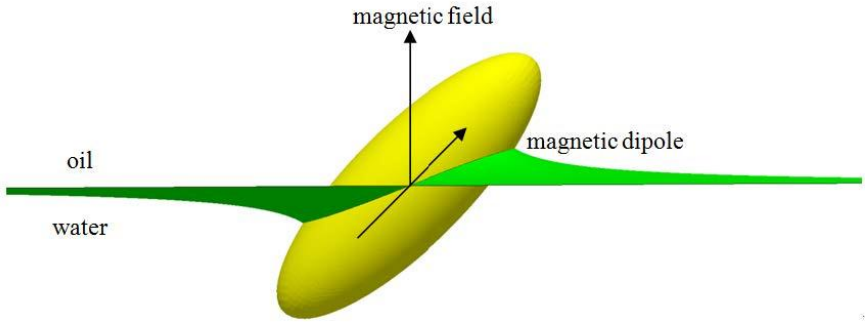

Figure 1: Surface Evolver image of an ellipsoidal particle adsorbed at a liquid interface in an external magnetic field perpendicular to the liquid interface.

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[2] C. Raufaste and S. Cox, Colloid Surface A 438 (2013) pp 126-131
[3] K. Brakke Exp. Math. 1 (1992) pp 141-165

Confined fluids and interfacial phenomena

P.19 Effective interaction between a colloid and a soft interface near criticality

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Within mean-field theory we determine the universal scaling function for the effective force acting on a single colloid located near the interface between two coexisting liquid phases of a binary liquid mixture close to their critical consolute point. Our semi-analytical approximation illustrates that from knowing only the profile of the interface, the force and the free energy can be accurately described. For a range of temperatures and capillary sizes, we find that for a colloid located more than 5 correlation lengths away the effective force between the particle and the fluid interface deviates less than 2% with that of a planar, rigid interface.

P.20 Adsorption energies of poly(ethylene oxide)-based surfactants and nanoparticles on an air-water surface

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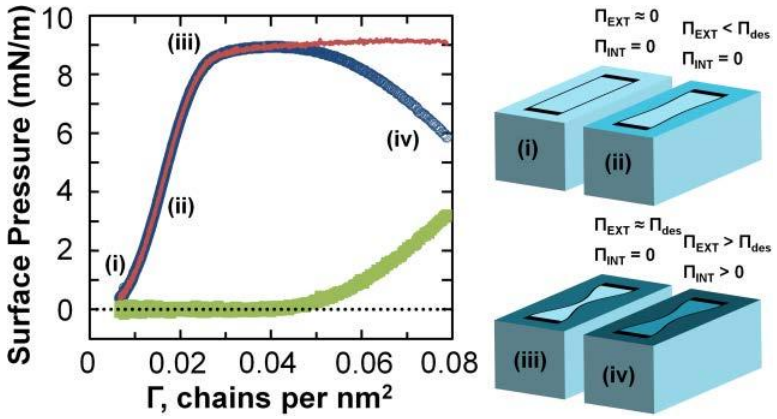
The self-assembly of polymer-based surfactants and nanoparticles on fluid-fluid interfaces is central to many applications, including dispersion stabilization, creation of novel 2D materials and surface patterning. Very often these processes involve compressing interfacial monolayers of particles or polymers to obtain a desired material microstructure. At high surface pressures, however, even highly interfacially-active objects can desorb from the interface. Methods of directly measuring the energy which keeps the polymer or particles bound to the interface

(adsorption/desorption energies) are therefore of high interest for these processes. Moreover, though a geometric description linking adsorption energy and wetting properties through the definition of a contact angle can be established for rigid nano or microparticles, such a description breaks down for deformable or aggregating objects. Here, we demonstrate a technique to quantify desorption energies directly, by comparing surface pressure-density compression measurements using a Wilhelmy plate and a custom-microfabricated deflection tensiometer. We focus on poly(ethylene oxide)-based polymers and nanoparticles. For PEO-based homo- and co-polymers, the adsorption energy of PEO chains scales linearly with molecular weight, and can be tuned by changing the sub-phase composition. Moreover, the desorption surface pressure of PEO-stabilized nanoparticles corresponds to the saturation surface pressure for spontaneously-adsorbed monolayers, yielding trapping energies of $\sim 10^3\ k_B T$.



P.21 Analysis of an axisymmetric two-phase flow model for particle transport at fluid interfaces

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The derivation of averaged equations describing bulk suspensions of particles has been the subject of a large number of studies (see e.g. [1]). In contrast, similar studies focusing on particles trapped at fluid interfaces, and whose trajectories are therefore constrained to lie on curved surfaces, are relatively scarce. The bulk of the literature indeed focuses primarily on interfacial transport of surfactants [see e.g.[2],[3]), which have specific features not found in colloidal systems and suspension of inertial particles, such as the importance of the particle size, the influence of gravity, and hysteretic effects in the surface pressure owing to deformation of kinetically trapped configurations. This talk examines similarities and difference between two-phase flow equations for bulk suspensions and interfacial suspensions. The analysis reveals that, apart from terms related to the curvature of the control volume, the governing equations for interfacial suspensions have the same structure as those for bulk suspensions. The essential difference is in the way the coupling terms are parameterized. In this talk, the issue of closing the particle-pressure term and the slip velocity for colloidal suspensions subject to lateral capillary and electrostatic forces [4,5] is explored using literature data. Simple closure models are proposed, and the resulting closed equations specialized to the case of a slender axisymmetric particle-laden interface. This case is amenable to mathematical analysis and is relevant to studies on the dynamics of axisymmetric liquid jets and bridges.

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Optical methods and imaging

P.22 Dual-mode microviscosity measurements in lipid monolayer and bilayer systems with a molecular rotor

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Viscosity of the cellular membrane has a significant impact on cellular processes, including on the diffusion of biomolecules within or through the membrane. Although measurement of viscosity on a microscopic scale is a challenging task, we have demonstrated[1] that it can be achieved with the aid of molecular rotors, which are fluorophores with viscosity dependent fluorescence intensities and lifetimes. Microviscosity measurements are usually performed via Fluorescence Lifetime Imaging Microscopy (FLIM), which produces a spatial map of the lifetime of a molecular rotor in the object of interest. Alternatively, ratiometric imaging can be used if the molecular rotor exhibits a viscosity dependent intensity ratio between two peaks in its fluorescence spectrum.

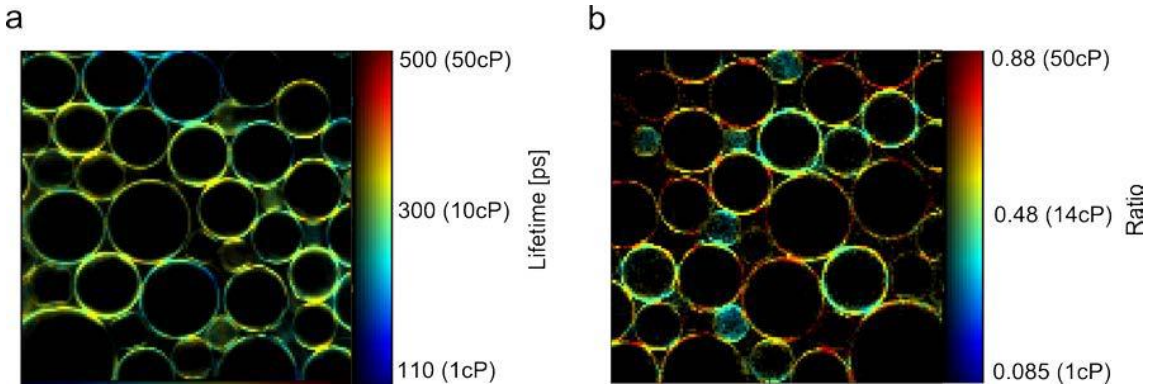

Figure 1. FLIM (a) and ratiometric (b) images of lipid monolayers around water droplets in dodecane. Viscosity values corresponding to the lifetimes and ratios given in the colourbar are shown in brackets.

In this work we have examined a molecular rotor MB, constructed as a porphyrin dimer, which is capable of measuring viscosity via both of the methods described above. Only a few such molecular rotors are reported in the literature, however, this provides a useful opportunity as it allows us to independently double check measured viscosity values. We performed the calibration of the rotor in methanol/glycerol mixtures of varying viscosity using both FLIM and ratiometric imaging (Figure 2). MB was then employed for measuring viscosity in several lipid-based systems, such as (i) lipid monolayers made by coating water droplets in dodecane with the lipid DOPC (Figure 1); (ii) large and giant unilamellar vesicles (LUVs and GUVs), which are used as model system for cell membranes.

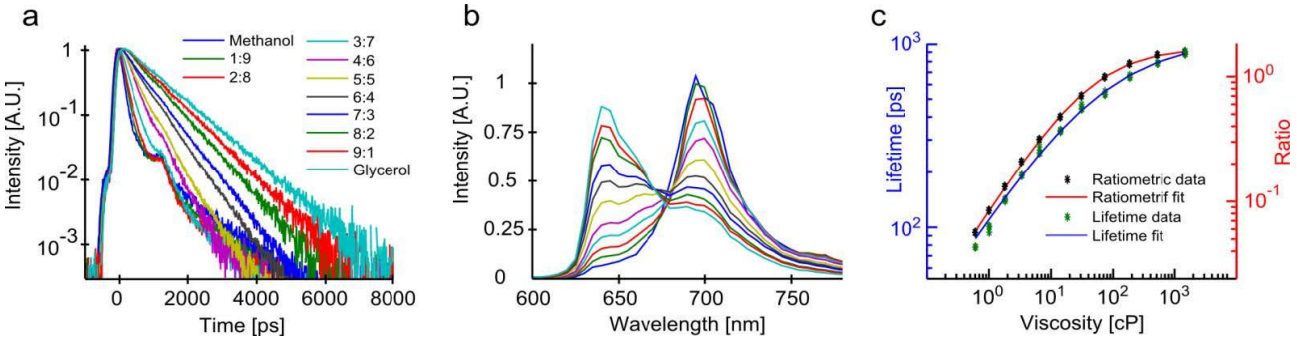

Figure 2. Calibration data of MB in methanol/glycerol mixtures. Normalized fluorescence decays (a) and normalized fluorescence spectra (b) in solvent mixtures of different viscosities. The volume ratios of glycerol to methanol are shown in the legend of (a). (c) Lifetime (blue) and ratiometric (red) calibration curves obtained from the data in (a) and (b).

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P.23 Imaging dynamic patterns in lipid membranes using molecular rotors

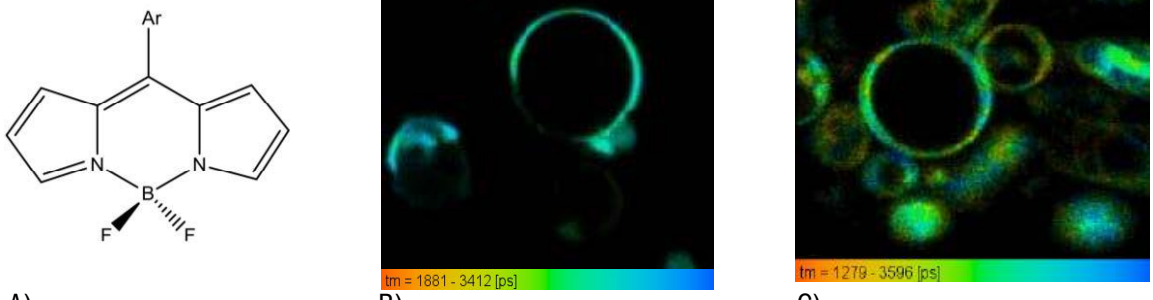
M R Dent, I Lopez-Duarte, J A Bull, N J Brooks and M K Kuimova

Department of Chemistry, Imperial College London, UK

The existence of ordered lipid microdomains within the plasma membrane of live cells has remained a contentious idea within the research community, partially due to the difficulty associated with optical imaging below the diffraction limit of visible light. By using a new imaging approach based on the use of molecular rotors and unilamellar vesicles as model membrane systems, we have developed a method capable of giving detailed information about the phase behaviour of lipids within a membrane to a high degree of spatial and temporal resolution.

Molecular rotors are synthetic organic fluorophores whose fluorescence properties are related to the viscosity of the surrounding environment. In highly viscous environments the emission intensity and fluorescence lifetime of the rotor will increase significantly. The fluorescence lifetimes of rotors based upon a boron-dipyrrin (BODIPY) core (Figure 1A) have been shown to have a strong dependence on the viscosity of the surrounding environment,[1] meaning that fluorescence lifetime imaging (FLIM) can be used in conjunction with BODIPY rotors to give a spatially resolved map of microviscosities across a sample, independent of the local BODIPY concentration.

Here we report the use of molecular rotors based on BODIPY to investigate membrane viscosity and phase behaviour within unilamellar vesicles using FLIM (Figure 1 B-C). We investigate the effects of lipid composition and temperature on observed viscosity values. We also use several synthetic derivatives of the BODIPY rotors with various functional groups in order to change the membrane localisation of the probes, e.g. the new charged derivative[2]. We examine the relationship between the measured viscosity and the BODIPY structure.



A) B) C)

Figure 1 Generalised structure of a BODIPY rotor (A), lifetime images of a phase separating ternary GUV stained with a BODIPY rotor at 29°C (B) and 45°C (C). Viscosity decreases with increasing temperature, and phase separation can be seen to disappear as the system is heated beyond the transition temperature of the lipids.

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P.24 A Label-Free Microfluidic Assay to quantitatively study antibiotic diffusion through lipid membranes

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The recent surge in numbers of antibiotic resistant bacteria has stimulated interest in the mechanisms of antibiotic transport across bacterial cell membranes. We present a label-free microfluidic assay that quantifies the permeability coefficient of a broad spectrum fluoroquinolone antibiotic, norfloxacin, as it diffuses across lipid membranes. We use giant unilamellar vesicles as a model system, tracking the diffusion of norfloxacin molecules into the vesicles using the UV autofluorescence of the drug. We directly obtain the permeability coefficient without requiring knowledge of the drug partition coefficient and validate theoretical predictions for the effect of pH on norfloxacin permeability. This technique can be further extended to quantify the effect of nanopores embedded in the membrane on drug diffusion.

P.25 Simple continuum descriptions of macromolecule complexes for imaging techniques

C Prior

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We have developed simple continuum techniques for describing thin electron densities in order to represent macro-molecular complexes. This description is appropriate for imaging techniques such as Small-angle scattering and fiber diffraction. The mathematical framework is significantly flexible. It allows for arbitrary shape,yields simple expressions for including repeat structures on the tertiary and quaternary scale and can allow for arbitrary levels of complexity of the density, including the facility to include solution-molecule interactions. It is particularly simple to describe structures composed of heilical units in this framework. In addition we have general expressions for the Fourier transform of these densities, which can be used to converted a predicted structure into a diffraction pattern. We introduce this framework and briefly mention recent and ongoing work applying these techniques to small angle scattering data.

Polymers, polyelectrolytes and biomolecules

P.26 Modifications of the study of dielectric properties of a polycarbonate plastic (Makrofol KG) induced by Si^{7+} heavy ion irradiation

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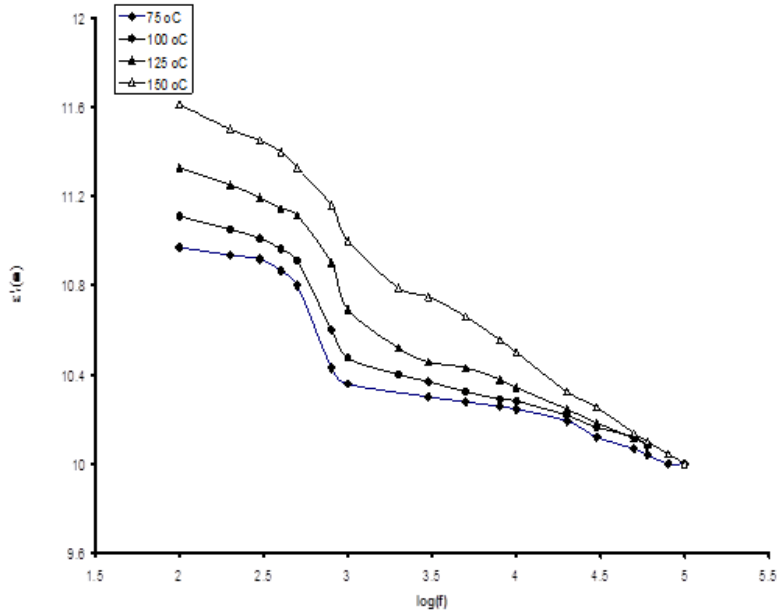
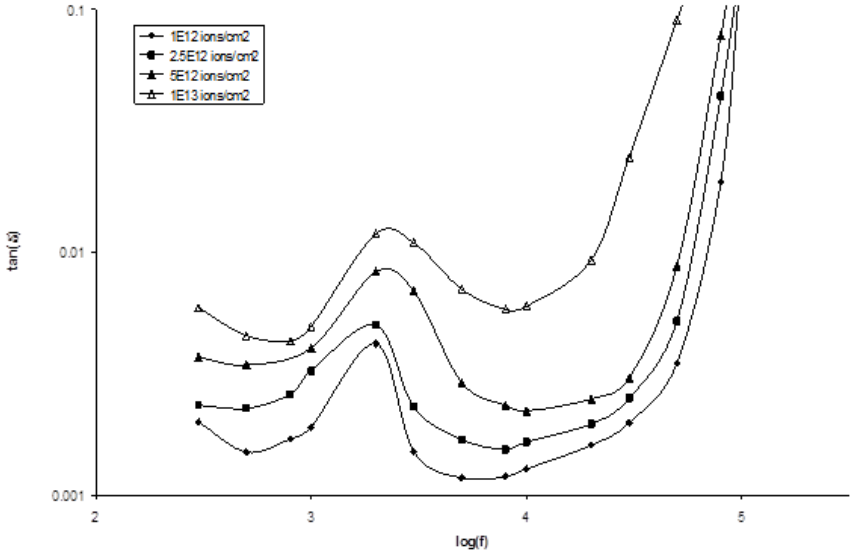
[1]Department of Physics, Faculty of Science, University of Tabuk, Saudi Arabia, [2]10+2 College, Aligarh Muslim University, India, [3]Department of Physics, Faculty of Science, King Abdul Aziz University, Saudi Arabia

When dielectrics, which have few free electrons, are placed in an electric field, polarization takes place and the electric dipole moments per unit volume are developed. The motion of the charge carriers in the insulating materials is very important at high temperature. Here, in this paper, we discuss using dielectric spectroscopy about the motion of the dipole movement and charge carrier, when dielectrics are subjected to alternating electric field. High energy heavy ion irradiation of polymers affects their dielectric constant and loss factor. Structural changes produced in the polymer owing to the breaking of its long molecular chains by heavy ions are responsible for such modifications in the polycarbonate plastic. Dielectric constant and loss factor are studied by irradiating samples with 100 *MeV* ^{28}Si ions with the fluence which varied from $1x10^{11}$ to $1x10^{13}$ ions/cm^2. The study is carried out for different frequencies of applied electrical field ranging from 1 k Hz to 100 k Hz and at various temperatures starting from room temperature to 125 ^{0}C both for the pristine and ion irradiated samples. We find that due to irradiation process polar

groups C=O and methyl group CH_3 became free and when they are subjected to the electric field, they rotate. We find two relaxation processes namely α and β one at frequency 20kHz and other at frequency 60 kHz. This relaxation is long range and localized. Their tan δ versus log f characteristic tells that the number of polymers taking part in the molecular motion increasesbecause of the increase in free volume. The activation energy in the case of pristineand *100MeV*^{28}*Si* ion irradiated samples was respectively found to be 102.1 kJ/mol and 74.4 kJ/mol.





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P.27 Pickering emulsion polymerized core-shell structured smart composite particles and their suspension rheology under electric and magnetic fields

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[1]Department of Polymer Science and Engineering, Inha University, Korea, [2]State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, China

Pickering emulsion, stabilized by solid particles instead of conventional emulsifiers, is an eco-friendly and facile way to prepare diverse functional organic–inorganic hybrid composites. Various solid particles such as exfoliated clay (including montmorillonite, laponite, etc.),[1, 2] silica nanoparticles,[3] and graphene oxide[4] have been reported as novel solid stabilizers in Pickering emulsions to fabricate hybrid particles for various potential applications. Recently, we have been working on core-shell structured magnetic polymers (polystyrene, poly(methyl methacrylate)/inorganic particles fabricated by Pickering emulsion polymerization using nano-sized Fe_2O_3 particles as a solid stabilizer, in addition to various inorganic particles such as clay and silica for electrorheological (ER) materials.[5-7] Figure 1 presents the SEM (a) and (TEM) images of the synthesized PS/Fe_2O_3 particles.[7] These core-shell structured composite particles are applied as smart materials for either ER or magnetorheological (MR) fluids,[8, 9] in which the ER/MR fluids are intelligent suspensions whose rheological properties can be well controlled with the external electric/magnetic stimulus. Their smart characteristics and rheological behaviors along with their Pickering emulsified fabrication will be covered.

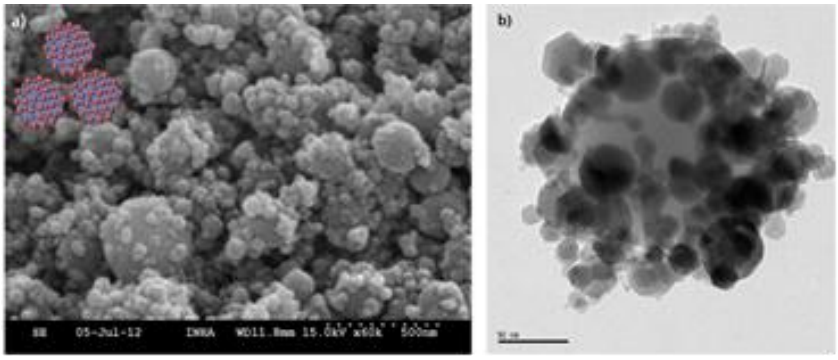

Figure 1 SEM (a) and TEM (b) images of PS/Fe_2O_3 particles by Pickering emulsion.

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P.28 Passive and active microrheology of a polymer melt studied by molecular dynamics simulation

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The rheological behaviour of a material is determined by the relaxation of its stress autocorrelation [1]. In simulation studies the stress tensor can explicitely be calculated and serves as a reference for the microrheological results, that are based on the behaviour of suspended particles [2]. The system under study is the well established bead-spring polymer melt model [3] including one or two nanoscopic particles.

Passive microrheology yields linear response properties of the polymer melt by looking at the thermal motion of the nanoparticles. From the mean squared displacement of the nanoparticles the complex modulus $G^*(\omega)$ of the melt is determined by using a generalized Stokes-Einstein equation. Results for different particle sizes, monomer-particle interaction strengths and temperatures are compared to the real microscopic moduli. With regard to hydrodynamic effects, a more complete form of the analysis is discussed [4].

For a comparison to recent experimental results from X-ray photon correlation spectroscopy [5], the temperature dependence of the incoherent intermediate scattering function is shown.

Furthermore the linear and nonlinear response of the polymer melt is investigated by applying forces to the melt (active microrheology). Here a nanoparticle-oscillator is used; i.e. two nanoparticles are connected by a harmonic potential and the compressed oscillator is put into the polymer melt. The resulting oscillation of the nanoparticles is studied for different melt temperatures and different spring constants.

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P.29 Microscobic probing of melting and gelation processes in well-defined biopolymer network

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Multiple particle tracking microrheology is used to study the melting and gelation behaviour of thermal responsive, telechelic, collagen-inspired polypeptide, TR4T, expressed by transgenic *P. Pastoris.* The system consists of a hydrophilic random coil-like middle block and collagen-like end blocks. Upon cooling, end blocks assemble into well-defined transient nodes with exclusively three-fold functionality. In this work, we demonstrate the master curves obtained from mean squared displacements of tracer beads by using the method of superposition introduced earlier for both melting and gelation processes. Melting point, gel point and critical relaxation exponents are determined from the shift factors. The use of dynamic scaling exponents to correctly determine the critical transition points is discussed. Critical relaxation exponents obtained for different concentrations in both systems are compared with the currently existing dynamic models in literature. Additionally, we demonstrate the strong dependence of critical transition points on concentration and compare the kinetics of both processes.

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P.30 Tunable reversible hydrogels from metal-coordinated polymers

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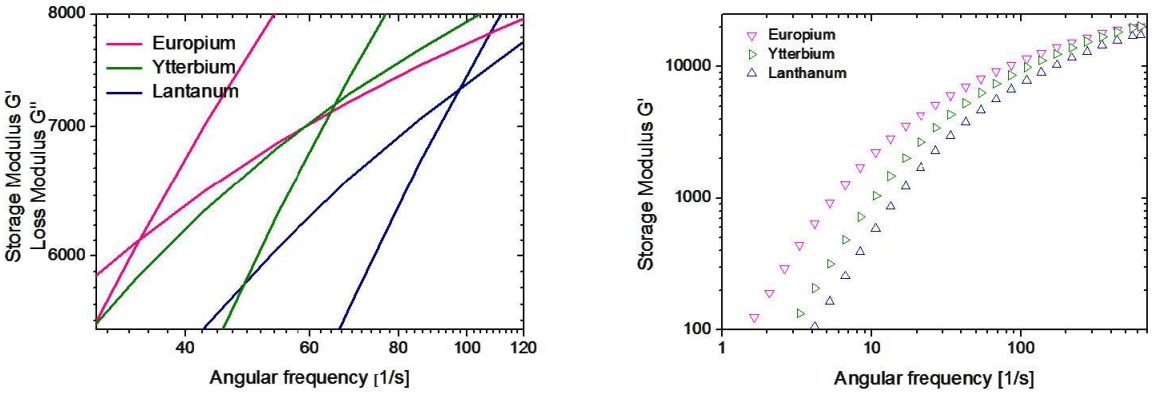
Here we present preliminary results of a systematic characterisation of a novel reversible and tuneable hydrogel materials formed by metal-coordinated linear polymers. These self-organizing structures have seen enormous innovation in recent years and they combine features of conventional polymer systems with electrochemical properties of metal-ligand complexes.

We use terpyridine-modified high-molecular-weight telechelic polymers, which in the presence of transition metal ions form linear supramolecular chains[1].

As the goal of this work is to form organometallic networks, the next step is to introduce lanthanide metal ions as an additional cross-linking elements[2]. In these systems, we can independently tune the degree of crosslinking, through changing the ratio between transition metal ions and lanthanide metal ions. Moreover, by choosing different metallic species we can tune relaxation time, which can vary from milliseconds to many days.



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P.31 Two-fluid model for ions distribution on a charged surface: A Monte Carlo study and modified Poisson-Boltzmann theory

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Department of Physics, National Changhua University of Education, Taiwan

It is generally believed that in the weak coupling regime, ion-ion correlation is not important, and then the mean field theory is valid. In the salt-free solution (with counterions only), the density profile of the counterions is the Gouy-Chapman solution. With salts, the mean field result is the Poisson-Boltzmann solution.

We investigate carefully the counterions and coions distribution on a charged surface in the weak coupling regime by the Monte Carlo simulation. It is found that the ions distribution does not fit into the Poisson-Boltzmann theory at the intermediate salt concentration. The ions distribution favor a two-fluid model in which the counterions are composed of two parts. One is bound (or called condensed) and the other is free (or called mobile).

Based on the simulation result, we propose a new kind of mean field theory, the modified Poisson-Boltzmann theory, for the two-fluid model. It is found that the theoretical result agree with the simulation.

P.32 The role of confinement and interaction range on polarisation and alignment of stiff chains and networks

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[1]Institute of Theoretical Physics/Department of Physics, Stellenbosch University, South Africa, [2]National Institute for Theoretical Physics, South Africa

Confining a stiff polymer chain to a compartment or pore influences the orientation of the bonds and density distribution of chain segments within the confining region. We utilise a formulation of the chain in terms of a monomer ensemble [1-3] to model the additional effect of an interaction between polymer segments at the mean-field level. In particular, we show how the interaction alters the effective stiffness as well as the spatial profile of the

location of segments. We analyse the respective roles of the interaction range and the confinement length scale to identify different types of behaviour for confinement. Our analytical results contrast confinement between parallel plates and restriction to spherical or circular pores. In additional to the analytical arguments we present results from simple molecular dynamics simulations of similar systems. The theoretical methods are also expanded to a formalism of a reversible, tree-like network. In this case variation of the confinement parameter permits a direct measure of elastic properties of such a finite and confined network. Aspects of these results are potentially applicable to some of the networks and chains found at cellular and sub-celluar levels.

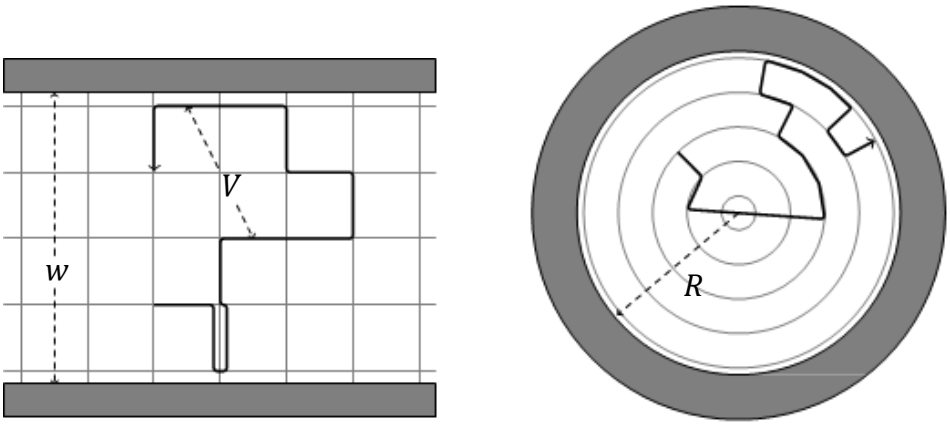

FIG. 1: On the left-hand side we show a sketch of a stiff, lattice-based chain confined between two parallel plates. We wish to determine the polarisation density in dependence of the interaction potential energy V between the bonds and the separation of the plates w. Spherical confinement is the second restricting geometry. We model the chain in a set of shells to derive the orientation profile in this region of radius R.

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P.33 Inert-tail effect on the thermodynamics of DNA hybridisation

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DNA hybridisation is the process by which double-stranded (ds)DNA is formed from two complementary sequences of single-stranded (ss)DNA. The hybridisation of short DNA strands is selective, reversible, and can be controlled by changing the temperature and ionic strength of the solvent. DNA-nanotechnology exploits these unique features to design supramolecular interactions for applications such as DNA-coated colloids [1], DNA origami [2], and biosensors [3]. The optimisation of these applications requires a quantitative description of thermodynamics of the hybridisation process.

The most common approach for predicting the hybridisation free energy between complementary ssDNA strands is based on the so called nearest-neighbour rules [4]: the free energy is decomposed into a sum of tabulated contributions associated to all the nearest-neighbour pairs of bases [gold beads in Fig. 1(a)], the “dangling bases” [red beads in Fig. 1(a)], and some initiation parameters.

However, in many practical applications of DNA-mediated self assembly the reactive “sticky ends” are connected to “inert” (non hybridising) DNA strands. Current models do not account for these “tail effects”.

We present experiments and simulations showing that the hybridisation free energy of DNA is significantly altered when the reactive bases are connected to inert tails [blue beads in Fig. 1(a)] [5]. The electrostatic repulsion between the tails and the hybridised section hinders the dimer formation. The binding strength becomes weaker upon increasing the number of tail bases and the ionic screening length. At physiological ionic strengths, the

nonspecific free energy shift is comparable in magnitude, but opposite in sign, to the contribution of a hybridised base pair. We show that the observed effects can be captured by a simple empirical formula that can be used to correct the nearest-neighbour predictions of the hybridisation free energies and melting temperatures.

(a)

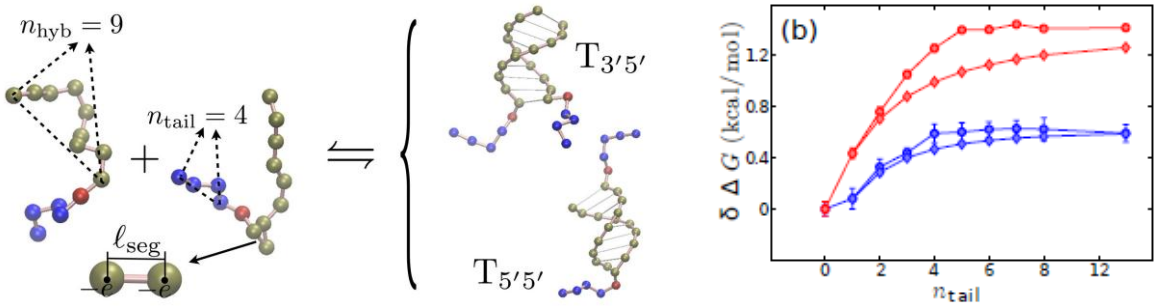

Fig. 1. (a) Hybridisation of two ssDNA strands with n_{hyb} complementary bases (golden spheres) and n_{tail} inert tail bases (blue spheres). The first dangling base, the contribution of which is included in traditional nearest-neighbour models, is depicted as a red sphere. Two architectures are investigated: $T_{5t\,5t}$ in which the tails are attached to opposite sides of the dsDNA, and $T_{3t\,5t}$, in which the tails are attached to the same side of the dsDNA. (b) Experimental (circles) and simulated (lozenges) free-energy shift ($\delta\Delta G$) as a function of n_{tail} for the $T_{5t\,5t}$ (blue) and the $T_{3t\,5t}$ (red) architectures.

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P.34 Large-area patterning of the tackiness of a colloidal nanocomposite adhesive by sintering of nanoparticles under IR radiation

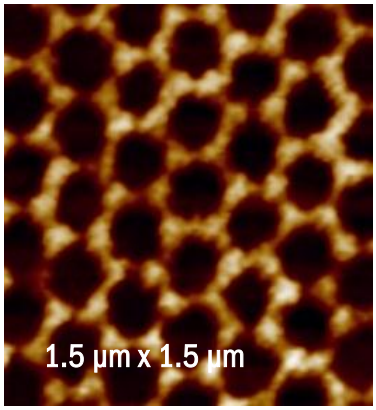
R Gurney[1], B Cooper[1], D Dupin[2], E Siband[3], K Ouzineb[3] and J L Keddie[1]

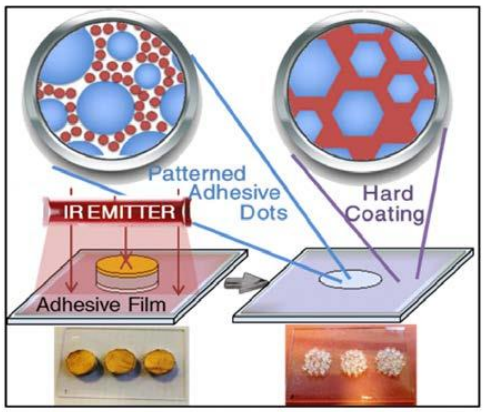
[1]University of Surrey, UK, [2]IK4-CIDETEC, Spain, [3]Cytec Surface Specialties, Belgium

Pressure-sensitive adhesives (PSAs) adhere instantly and firmly to a substrate upon the application of a light pressure. PSAs require the right balance of elastic and viscous properties.[1] A high adhesion energy results not only from the thermodynamic work of adhesion at an interface with a substrate, but also from the bulk mechanical properties, including the large-strain deformation behaviour.[2] With increased emphasis on recycling and re-use of materials, there is interest in adhesives that de-bond or “switch off” on demand, when triggered by an external stimulus. There is a growing need for adhesives that are patterned such that only a portion of their surface is tacky. For instance, electronic components must be attached at specified positions on a PCB, on which electrically conductive adhesives replace metallic solders.

We present a simple technique to switch off the tack adhesion in selected areas of a waterborne colloidal nanocomposite adhesive layer.[3,4] Blends of glassy polymer nanoparticles and larger, soft colloidal particles are cast to create a nanostructured film (see figure, on the left). During probe–tack testing, the soft polymer phases yield and enable fibrillation. After heating under IR radiation, the nanoparticles sinter together to make a rigid percolating structure. The storage modulus increases by a factor of five, and the yield point increases nearly by a factor of six, such that yielding and fibrillation do not occur in the probe–tack tests. In regions that are exposed to IR

radiation through a mask, such as gold-coated coins (shown here on the right), the nanoparticles sinter together and harden the adhesive, thereby destroying the tack adhesion locally. Adhesive island regions are defined with the surrounding regions being non-tacky. The process enables switching of the adhesive surface at a desired position.[4]





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P.35 Lubrication by polymersomes under nanoconfinement

J E Bartenstein[1], J S Diget[2], B Ø G Nystrøm[2], P M Claesson[3] and W H Briscoe[1]

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Polymersomes, which are hollow spheres made from amphiphilic block copolymers, have been widely studied in literature for applications in biomedical sciences, *e.g.* as drug carriers and artificial cells, but no research has been reported on their lubrication properties. They show a close resemblance with liposomes including their hydration behaviour, however, polymersomes generally have a higher stability which, we hypothesise, makes them promising materials for lubrication applications.

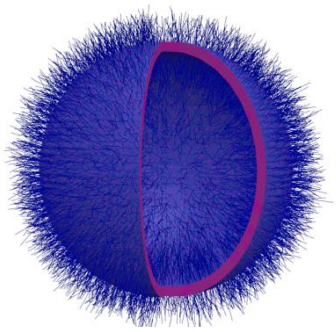

Figure 1. Schematic presentation of a polymer vesicle.

An effective friction reduction mechanism is *hydration lubrication*. Here water molecules in the primary hydration layer are bound tightly to ions and thus able to support load. Meanwhile, they are in rapid exchange with free water molecules, giving rise to a fluidity of bound water molecules similar to that in bulk, facilitating lubrication under pressure. We hypothesise that hydrated polymersomes can mediate a similar mechanism.

To this end, colloidal probe atomic force microscopy (CP-AFM) is used to study the characteristics of polymeric assemblies under confinement and shear. Initial CP-AFM experiments on PBD-PEO polymersomes in water show that the polymersomes are very "slippery" and facilitate low friction coefficients. Additionally, their morphology on a surface was studied by AFM imaging in a liquid cell.

From these observations, we hypothesise that polymersomes are promising candidates as biomimetic synthetic lubricants. We will make direct measurements of surface forces, particularly friction, mediated by different polymersomes with sizes between 50-400 nm self-assembled from a range of copolymers using the surface force apparatus.

Rheology and non-equilibrium phenomena

P.36 Spatio-temporal dynamics of collective flow across a bacterial carpet

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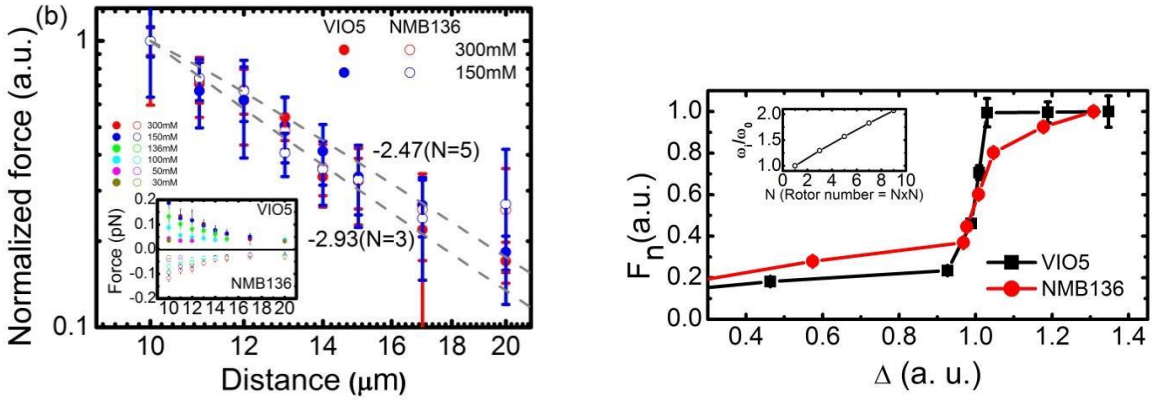
We investigate the spatio-temporal dynamics of collective flow across an array formed by self-propelling particle (SPP) (bacterial carpet) under low Reynolds number (Re) condition. Bacterial carpets consist of randomly anchored single polar-flagellated bacteria matrix are prepared by flow deposition. Collective flow across the bacterial carpets are probed with optical tweezers-microsphere assay. For two different bacterium strains of single polarly-flagellated *Vibrio alginolyticus* (VIO5 or NMB136), forces that pull (push) microsphere towards (away from) carpet are detected at distance > 10μm away from carpets. The normalized force curves scale between $r^{-2.5}$ to $r^{-3.0}$. Numerical calculation considering hydrodynamic coupling suggests the detected forces are superposition of fields from anchored force monopoles and their associated image flow fields. At flagellar rotation rate over a critical value, the force magnitudes increase abruptly. The observation suggests onset of hydrodynamic synchronization across bacterial carpet may be a threshold-like process. Implementing a high temporal resolution position sensitive photodiode enables us to investigate the synchronization phase slip dynamics under various sodium-motive driving conditions. We further explore the interplay between hydrodynamic interaction and thermal noises with respect to the cluster size and the temporal evolution of the flow field domains.



P.37 Surface roughening due to patchy particles in (1+1) dimensions - A computational study

M J Kartha and A Sayeed

Department of Physics, University of Pune, India

In recent years new extraordinary material synthesis techniques have been developed, which have made possible the fabrication of so called 'patchy' particles - particles of nanometers to micrometers sizes, which have inhomogeneous or 'patchy' surfaces. They interact mutually through highly directional, short range forces, and are capable of aggregating into very novel structures. We have carried out a computational study of the ballistic deposition of model patchy particles in 2D. This study simulates the physical processes where particles are

projected on to a substrate and undergo deposition to form a cluster. In our study the particles interact with each other through highly directed, strong and short range forces. This is done using the so called Kern-Frenkel model. We found that the growth process shows a phase transition which occurs at a critical patch size of $p_c = 0.6454$. For adhesive patch sizes below a well-defined critical value the growth of cluster kinetically terminates. That is, the cluster essentially stops growing, because the growth becomes stochastically improbable and we have a 'blocked' phase. For patch sizes above the critical patch size the aggregation continues indefinitely, which is a 'growing' phase. We have studied the changes in the growth process, the surface morphology of the clusters for varying patch sizes. The surface morphology of the cluster in the growing phase well above pc is that of a typical ballistic growth, which is characterized by a surface roughness $w(t)$ that increases as t^{β} for $t << t_x$, and remains constant for $t >> t_x$, where t_x is known as the cross-over time and β the growth exponent. For ballistic deposition of homogeneous particles $\beta \approx 0.33$ and we also obtain similar values. We obtain a dramatically different morphology for patch sizes near p_c, that is, in the critical region like the growth of a fractal, tree-like structure to mushroom like structures. In the critical region, the surface width values is found to be much higher than the normal ballistic deposition model and the growth exponent dramatically deviated than from the expected KPZ prediction. Recent studies on deposition of highly anisotropic particles near at air-water interface appear to belong to KPZ class with quenched disorder. Our study also appears to be similar to the growth of the interface due to pinning effects. Our study gives an insight for understanding the kinetic roughening of the growth species with anisotropic interactions.

FIG. 1. (a)Growth of interface width with time for BD model for a system of patchy particles for different patch size(b)The surface morphology of the film for the patch size $p = 0.6$. The tree like growth of the surface is observed.

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P.38 Lipid bilayer membranes under shear flow from molecular simulations

A Botan, L Joly and C Loison

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According to the World Health Organization every tenth person in the world suffers from joint pain associated with arthritis. In this disease there is a disturbance in regeneration of tissues which prevent direct contact of bones making up the joint. Particularly, the deficiency of synovial fluid causes stiffness and pain as well as destruction of cartilage. The point is that synovial fluid reduces friction between the articular cartilage of synovial joints during movement to extremely low values (0.005-0.04), that is much lower than values attained using any synthetic bearing materials in equivalent situations. To explain these values, a fluid film mechanism, where the two sliding surfaces are separated by a thin hydrophobic layer of the lipid bilayers (a component of synovial fluid), has been proposed. The molecular structure of the lipids, their organization, hydration level are called the major factors responsible for such low friction. To quantify their influence we model lipid bilayers under a shear using non-equilibrium molecular dynamics simulations (NEMD). In this approach, water is confined between two lipid bilayers, and the shear flow is induced by moving the top and bottom membranes in opposite directions at constant velocity. Molecular configurations are then used to provide insight into the interactions of lipids with water. The results are compared with experimental data.

P.39 The tube axis and entanglements in polymer melts

A Likhtman

University of Reading, UK

Although the tube theory is very popular and successful, the tube concept remains evasive and ill defined. In the first part of this talk I'll describe a simple computer algorithm to construct the tube axis as a center line of the cloud of chain configurations at different moments of time. We test this algorithm on trajectories generated from simulations of concatenated well entangled ring polymers, thus avoiding all disentanglement processes. We find that entanglements are clearly manifested through the curvature of tube axis, and we can succesfully identify binary and ternary entanglements in molecular dynamics simulations. Several quantitative characteristics of entanglements are reported and discussed. The second part of this talk will discuss a definition of entanglements as persistent contacts between the mean paths of polymer chains. This definition will be tested in molecular dynamics simulation of linear melts. We trace the dynamics of individual entanglements and study their lifetime, distribution along the chain and the way they are created or destroyed.

Self-assembly, biomimetics and pattern formation

P.40 From wound healing to artificial muscles: Modelling bio- and biomimetic materials with polar and nematic order parameters

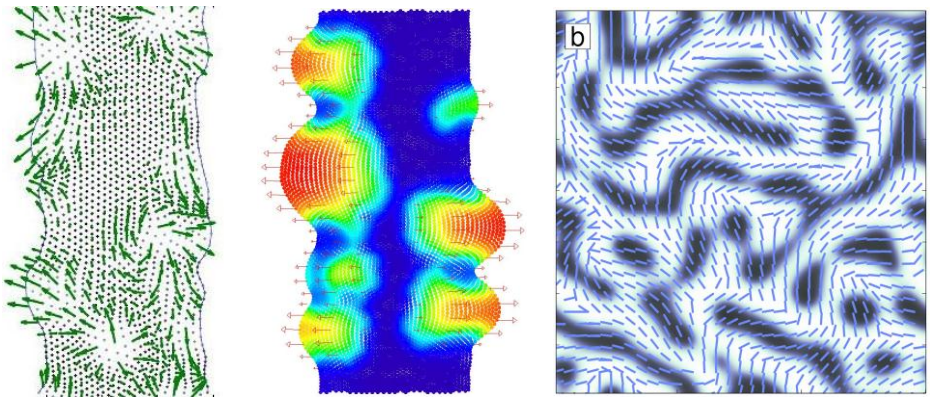
M H Koepf[1,2] and L M Pismen[2]

[1]Département de Physique, Ecole Normale Supérieure, France, [2]Department of Chemical Engineering, Technion, Haifa, Israel

Many biological and biomimetic materials can be described using continuum models with polar or nematic order parameters and nonlinear elasticity. Several examples will be given in this talk.

During unconstrained spreading as occurs for example in wound healing, epithelial cell monolayers can be described as polarizable and chemomechanically interacting layers with weakly nonlinear elasticity. Our model reproduces the experimentally observed self-organized formation of finger-like protrusions due to the collective action of a large number of cells [1,2]. Statistics of the velocity orientation shows a strong alignment in the fingers opposed to an isotropic distribution in the bulk, in agreement with measurements by Reffay et al. [3]. The model further captures the stress accumulation within the tissue that proceeds in form of a “mechanical wave”, originating from the wound edge [4].

A very similar model can be used to describe liquid crystal elastomers. These materials, whose flexibility and mechano responsiveness mimics biological tissues, can be used to construct actuators operating as artificial muscles. We focus on the case of elastomers doped with isotropic components and show how the coupling between the dopant concentration and the nematic order parameter influences the shape and orientation of domains formed during the demixing process [5].



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P.41 Dynamical Landau theory for the assembly and disassembly kinetics of supramolecular polymers

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Theoretical studies of the kinetics of supramolecular self-assembly are in general based on reaction-rate master equations, which are usually nonlinear and very difficult to solve analytically.

Hence, we attempt to describe these processes in a different way using only two moments of the full distribution of sizes of the assemblies.

For co-operative self-assembly these moments show very large yet not quite diverging susceptibilities, allowing us to write down a Landau-type free energy function satisfying conditions obtained from equilibrium statistical mechanics of self-assembled supramolecules. This free energy function then naturally leads us to evolution equations for the relevant order parameters, which are the two relevant moments of full distribution being the average degree of polymerization and the fraction of active material accounting for nucleated self-assembly.

Solving these differential equations, we are able to describe experimentally observed phenomena, including as overshooting, hysteresis and a lag time to assembly.

P.42 Engineering DNA-linked janus liposome clusters towards applications in drug delivery

T Wild

University of Leeds, UK

We aim to develop controlled liposome clusters as potential multi-drug carriers for application in nanomedicine therapies. To this end, we are utilising a platform where different liposomes can be connected through DNA linkers, to deliver multiple species keeping the individual cargos separate. Liposome clusters can be formed using complementary saturated lipid DNA conjugates integrated into the liposome's surface. To ensure strong and directional liposome bridging, a patch of localised DNA will allow assembly of size-limited clusters due to the directionality of the adhesive interaction. Previous studies have localised DNA on the surface of a liposome though phase coexistence, where the mixing of saturated (DPPC) and unsaturated (DOPC) lipids with cholesterol lead to the formation of liquid ordered patches of saturated lipid, surrounded by a liquid disordered phase of unsaturated lipids [1]. However these studies display poor saturated lipid DNA partitioning to the liquid ordered patches, allowing unwanted weak DNA hybridisation between the liquid disordered phases [2]. Therefore to enhance saturated DNA partitioning to the liquid ordered phase cardiolipin (CL) was added. CL is a highly unsaturated lipid which adopts a negative curvature, 10 mole percent has been shown to increase saturated lipid DNA partitioning by an order of magnitude [2]; driven through CL increasing the free energy required for a saturated lipid to insert into the liquid disordered phase. However the addition of CL requires a new four component phase diagram to be plotted, where tie lines across the liquid-liquid coexistence region determine the relative domain sizes and hence the size of the adhesion plaques. Due to the nanoscale liposome size required for cellular uptake, we use liposome diameters of 100 nm, prohibiting the use of optical techniques to view the phase separation. Therefore to map out the four component phase diagram we use a Förster Resonance Energy Transfer (FRET) fluorescence spectroscopy technique, which reports the redistribution of dyes during phase separation due the change in mean inter-probe distances. We are investigating the cluster size formed between two populations of Janus liposomes as we vary the relative domain size of the DNA-functionalised phase. This platform will be further developed towards targeted drug delivery of combination therapeutics, for example to combat multi-drug resistance or to deliver prodrugs with an activating compound.

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P.43 All-optical manipulation of photonic membranes

B Kirkpatrick[1], M Ploschner[2], M Damodaran[1], T Čižmár[2] and A Di Falco[1]

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We use an inverted holographic optical tweezers scheme, as shown in figure 1a), to all-optically manipulate and actuate photonic membranes, with engineered opto-mechnical responses. Photonic membranes based on hybridization of metallic nanofeatures on polymeric substrates have already been shown to make precise, robust and flexible optical filters [1], which can be made compliant to complex shapes, like the tips of optical fibres[2]. This makes them particularly well suited to biophotonics application, due to their precise sensing capabilities and highly flexible nature [3,4]. Optical tweezers are a precise manipulation tool for translating and orienting photonic membranes within biological samples, unlocking intriguing applications.

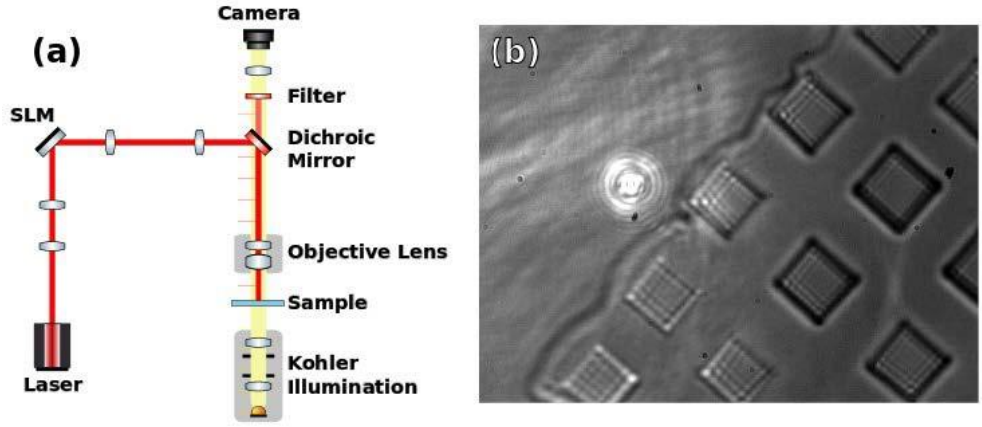

Figure 1a) shows schematic diagram of the inverted optical tweezer scheme used to manipulate extended polymeric membranes like that shown in figure 1b). Membrane show in figure 1b) had side length on the order of 100 μm.

Here we present and discuss preliminary results obtained for the all-optical manipulation of extended (edge length ~ 100 μm) SU8 polymer-based membranes like those shown in figure 1b).

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P.44 Self-assembly of nanoparticles on fluid membranes

A Saric

University of Cambridge, UK

We show how fluid membranes can mediate linear aggregation of spherical nanoparticles binding to them for a wide range of biologically relevant membrane rigidities. This result is in net contrast with the isotropic aggregation of nanoparticles on fluid interfaces or the expected clustering of isotropic insertions in biological membranes. We find that the key to understanding the stability of linear aggregates resides in the interplay between bending and binding energies of the nanoparticles. Furthermore, we demonstrate how linear aggregation can lead to membrane tabulation and determine how tube formation compares with the competing budding process. The development of tubular structures requires less adhesion energy than budding, pointing to a potentially unexplored route of viral infection and nanoparticle internalization in cells.

P.45 Inherent variability in the kinetics of autocatalytic protein self-assembly

J Szavits-Nossan, K Eden, R J Morris, C E MacPhee, M R Evans and R J Allenz

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The self-assembly of protein molecules into amyloid fibrils is associated with many degenerative diseases [1], but also presents potential opportunities for the development of new materials [2]. Kinetic experiments present an important tool in unravelling the mechanisms of filamentous protein self-assembly, yet replicate experiments often show significant variability [3-5], which is not accounted for in deterministic models [2, 6, 7]. Here, we introduce a stochastic model for autocatalytic filamentous protein self-assembly that includes primary nucleation, irreversible filament elongation and autocatalysis via fragmentation (see Fig. 1). Our main result is a prediction for the full distribution of lag times arising from intrinsic molecular noise, which we compare with experimental results for the aggregation of bovine insulin (see Fig. 1). Our findings show that stochastic effects cannot be neglected in small volumes, which are of most interest as they are comparable to the volume of a human cell.

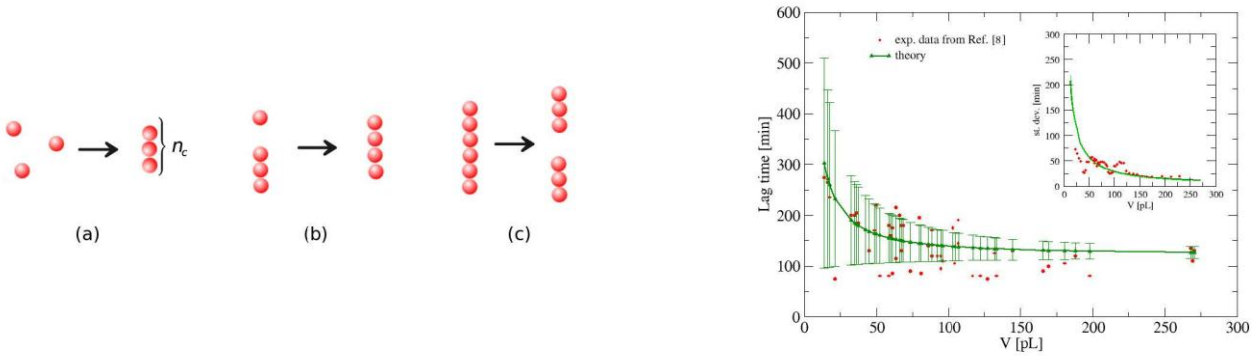

FIG. 1: Left: Schematic illustration of: (a) primary nucleation, (b) elongation via polymerization and (c) fragmentation. Critical nucleus size for primary nucleation is denoted by nc. Right: Theoretical prediction for the mean lag time in small volume samples (with standard deviation as error bars), compared to the experimental data from Ref. [8]. Inset: Volume dependence of standard deviation as predicted from the stochastic model, compared to experimental results from Ref. [8].

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P. 46 Understanding the self-assembly and structure of interfacial films formed from the bacterial hydrophobin BslA

R J Morris[1], K M Bromley[1], G Brandani[1], M McCluskey[1], D Marrenduzzo[1], U Zachariae[2], L Hobley[3], N R Stanley-Wall[3] and C E MacPhee[1]

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The protein BslA is physiochemically similar to the well-known surface active fungal proteins, hydrophobins, and may be regarded as a new class of bacterial hydrophobin. *In vivo*, BslA confers surface hydrophobicity to *B. subtilis* biofilms which may contribute to the protective qualities of the biofilm. Purified BslA spontaneously self-assembles at interfaces *in vitro*, forming an elastic film. We use pendant drop tensiometry, electron and confocal microscopy, and circular dichroism spectroscopy coupled to molecular dynamics simulations to understand both the structure and assembly of these interfacial films. We find that wild type BslA assembles into highly ordered 2D rectangular lattices which, upon self-assembly, contain long-range beta-sheet structure. Molecular dynamics simulations shed further light on the molecular mechanisms of BslA interfacial assembly.

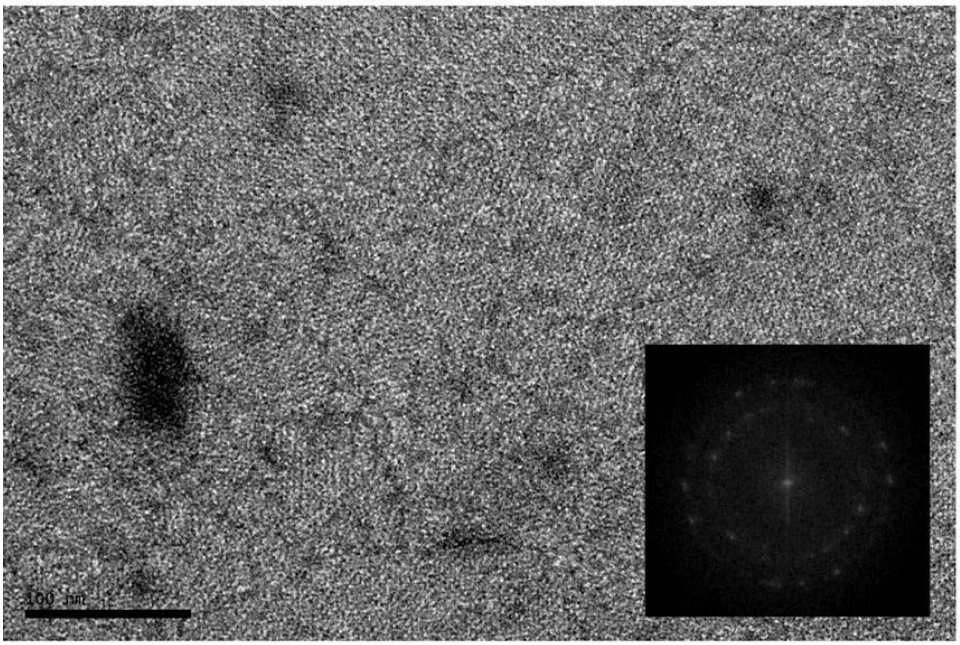

Fig. Wild-type BslA film imaged via TEM. Inset shows FFT of entire TEM image. Scale bar is 100 nm.

P.47 Self-assembly of naphthalene-dipeptides to form hydrogel films at the air-water interface

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Supramolecular gels from the self-assembly of peptide amphiphiles are widely used for a range of technological applications, such as controlled drug release, cell culture, template materials and tissue engineering. Gelation can be introduced by decreasing the pH, which protonates the carboxylic acid and make the molecular more hydrophobic. Compared with bulk hydrogel, thin films of assembled peptides have higher thermal stability and mechanical durability, and also open the possibility of studying their interfacial properties. In my experiments, different naphthalene dipeptides (NapFF and BrNapFF) have been successfully trapped at an air-water interface by depositing the dipeptide solution onto a low pH subphase. The mechanism for interfacial trapping has been studied.

Both FTIR spectra and AFM images are used to research the structure of these films. In addition, measurement using a Langmuir trough shows that these films are elastic. Finally, these films are able to stabilize large air bubbles for several days.

Surfactants, foams and emulsions

P.48 Dynamic wetting of hydrophobic polymers by aqueous surfactant and superspreader solutions

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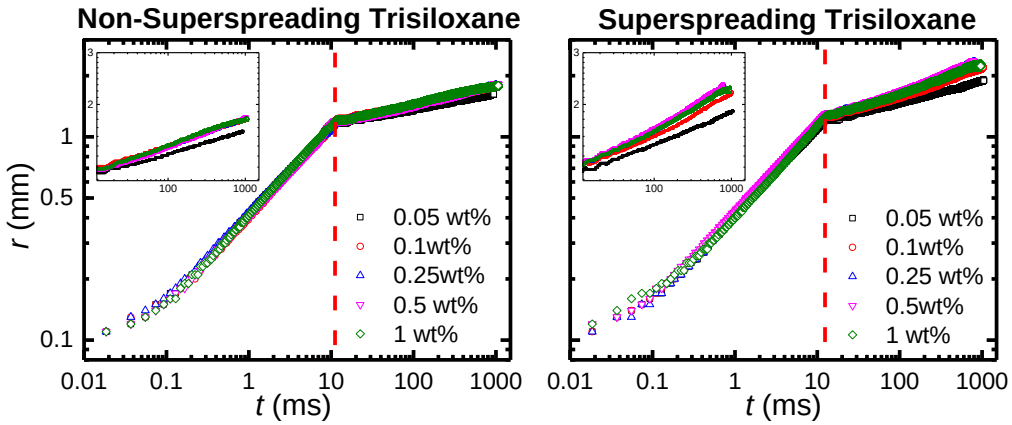
We carried out a systematic study on the wetting dynamics of aqueous solutions of conventional ionic surfactants (CTAB, SDS) and nonionic trisiloxanes (TSS10/2, TSS6/3) with different concentrations on hydrophobic polypropylene substrates. We showed that – depending on the surfactants – one, two, or three stages of dynamic wetting occurred, and that each stage was described by power law dynamics. For all surfactant solutions, the early wetting stage was dominated by inertia and the duration of this stage was not influenced by the presence of surfactants. For CTAB and SDS solutions, only this wetting stage was observed. For both trisiloxanes, after the inertial stage we observed a second viscosity-dominated wetting stage. In this stage, TSS10/2 showed an enhanced wetting capability independent of its concentration, while TSS6/3 started to show a concentration-dependent spreading behavior that was fully developed in a third "superspreading" stage. Our findings suggest that the superspreading property of TSS6/3 began to take effect after a characteristic time, before which the superspreading TSS6/3 and the non-superspreading TSS10/2 behaved similarly. Power law fits to the superspreading regime are in agreement with an interpretation of Marangoni flows resulting from surface tension gradients.



Log-Log plots of spreading radius *r* vs. time *t* of aqueous drops of non-superspreading and of superspreading trisiloxane solutions on polypropylene. Insets zoom in the spreading data in the second stage.

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[2] J. Venzmer, Curr. Opin. Colloid Interface Sci. 16, 335(2011)

P.49 Atomistic description of the solubilisation of testosterone propionate in a sodium dodecyl sulfate micelle

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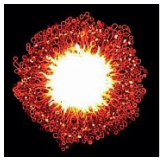
Amphiphilic molecules consist of polar head groups and nonpolar tails. Due to this chemical composition, amphiphilic molecules are known to self-assemble into a variety of aggregate structures in aqueous solutions, including micelles, bilayers, vesicles and lamellae. In all of these aggregate structures, the hydrophobic (nonpolar) parts of the molecules assemble to form an apolar interior of the aggregate, from which water is expelled, and the hydrophilic head groups of the molecules are found at the aggregate/water interface. The hydrophobic microenvironment that results from the aggregates in solution can be used to enhance the aqueous solubility of other slightly soluble nonpolar substances. This phenomenon is called "solubilisation". The solubilisation of molecules plays an important role in a variety of industrial and biological processes (including the design of cleaning agents, cosmetics, & pharmaceuticals). Despite the broad application of micelles for solubilisation, the molecular picture of the solubilisation process is not well understood.

In this presentation, we will report the results of molecular dynamics simulations in which we study the solubilisation of testosterone propionate in sodium dodecyl sulfate (SDS) micelles. SDS is a commonly used amphiphilic molecule in the pharmaceutical formulations, which has a twelve carbon hydrophobic tail and an anionic headgroup. We have conducted molecular dynamics simulations of SDS micelles with and without testosterone propionate in an aqueous solution. We will report on how the presence of the drug molecules in the micelles affects the structure, size and shape of the SDS micelle. As the drug molecules are solubilized by the the SDS micelle we will investigate how the interfacial properties of the SDS micelle alters, and also how the solvation of the drug molecule changes. Finally, we will provide a detailed description of solubilisation process of the testosterone propionate, and in turn provide a description of the atomistic interactions, which govern this process. Where appropriate these results will be compared to and verified with the results from small angle neutron scattering experiments.



The Physics of Soft and Biological Matter

Poster Session B

Biological systems

P.01 Force localization in contracting cell layers

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A primary mechanism by which cells sense the mechanical properties of their environments is by exploiting the contractility of their internal cytoskeletal networks to 'pull' on the external gel. For single cells, the strength of this pulling force is traditionally measured using Traction Force Microscopy (TFM). In TFM the amount that a cell displaces the gel is carefully measured and correlated to the mechanical activity of the individual cell [1]. However in tissues, interpreting these results is significantly complicated and usually we are left to infer the magnitudes of cellular forces through indirect methods such as by mechanical relaxation after laser cutting [2].

We here present a different approach, using theoretical modelling to interpret tissue level experimental observations. We develop a continuum elasticity model for a TFM experiment of a contractile epithelial cell sheet on an underlying gel substrate [3]. This model is used to show how the observation of greater displacement at the sheet edges can be explained by uniformly contractile cells rather than necessarily implying increased mechanical activity at the edges as has often been assumed. We show that the observed profiles of displacements is determined by a single non-dimensional parameter and that this parameter interpolates between linear and exponential force profiles for the extreme cases of very soft and very stiff substrates, respectively. If contractility is sufficiently increased at the periphery, we predict that outward directed displacements can occur at intermediate positions, although the edge itself will still retract. We also show that anisotropic extracellular stiffness leads to force localization in the stiffer direction, as observed experimentally.

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[2] Hutson, M. S. et al. *Forces for Morphogenesis Investigated with Laser Microsurgery and Quantitative Modeling*. (2003) Science 300(145) 145-149

[3] *Edwards, C.M. and Schwarz, U.S. *Force localization in contracting cell layers.* (2011) Phys. Rev. Lett. 107, 128101. (**Author* C.M. Dunlop - published under maiden name of Edwards)

P.02 Orientational order and motility in active droplets

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Spatially confined active matter exhibits fascinating collective behaviour, for instance internally generated flows in, and macroscopic self-propelled motion of active fluid droplets. Both seem to be associated with a particular long-range orientational order of the active particles in the droplet.

Our aim is to understand which type of orientational order enables the transmission of local activity onto large scales and leads to directed movement of the drop. We consider a three dimensional drop of active matter that has a fixed, flat shape and is located on a plane surface. We impose different orientational fields with topological defects and calculate the resulting flow fields inside the drop analytically by solving the Stokes equation, which

contains an active stress. For certain cases we show that an asymmetry in the imposed orientation field is inherited by the flow and enables motility in the case of appropriate boundary conditions at the contact surface.

One example of an active droplet is a cell extract, that is a solution of active cytoskeletal compartments confined by the cell membrane. Thus, understanding the interplay of orientational order and directed macroscopic movement could reveal new insights into the basic mechanisms of cell motility.

P.03 Fluctuating finite element analysis: Modelling biomacromolecules with continuum mechanics

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We present a recently developed, novel method for coarse grained simulation of dynamics of globular proteins. We use a continuum mechanics description of the proteins, solving this using a Finite Element algorithm which we have generalised to include thermal fluctuations, and which is therefore known as Fluctuating Finite Element Analysis (FFEA) [1]. One advantage of this approach is that it permits simulations of molecules those for which no experimental atomistic level structure exists, but for which data is available on the mesoscale shape, and flexibility, of the structure. For example, biophysical techniques that provide such information include cryo-electron microscopy and 3D tomography, which are now sufficiently mature that they merit their own online repository called the EMDataBank (EMDB).

Our method is still in its infancy: we are still developing aspects of the model to include different physical processes. Nevertheless, we have begun to explore biological applications. FFEA has been used to calculate the principal modes of V and A type ATPase membrane motors for comparison with experimental flexibility data, and to produce a quantitative comparison with the results of the Elastic Network Model for the same system. FFEA has also been used to simulate the dynamics of the largest cytoskeletal motor, dynein, in both the APO and ADPVI stages of its power stroke. We have investigated how the crowded environment of the axoneme impedes dynein's thermal fluctuations and the corresponding effect on its exploration of the microtubule surface, allowing us to produce an estimate of the motor's step size *in situ*. We are currently applying the FFEA model to inform the design of biosensors by quantifying how protein flexibility affects binding and unbinding rates from an adhesive surface.

[1] R. Oliver, D. J. Read, O. G. Harlen and S. A. Harris. *J. Comp. Phys.* 2013, 239 147-165

P.04 Dynamics of oblate and prolate capsules in shear flow

Z Wang[1], Y Sui[1], P D M Spelt[2,3] and W Wang[1]

[1]School of Engineering and Materials Science, Queen Mary University of London, UK, [2]Laboratoire de Mécanique des Fluides & d'Acoustique (LMFA), CNRS, France, [3]Département Mécanique, Université Claude Bernard Lyon 1, France

The dynamics of oblate and prolate spheroidal capsules in simple shear flow with a small inertia is studied numerically for a range of dimensionless shear rates. The capsule is modelled as a liquid droplet enclosed by a hyperelastic membrane, and its equatorial plane is initially tilted out of the plane of shear. At low dimensionless shear rates, it is found the well accepted tumbling motion is not always stable for both oblate and prolate capsules. For an oblate capsule, the dominant stable modes for increasing dimensionless shear rate are as follows: rolling with the equatorial plane staying in the plane of shear, precessing following Jeffery's orbit [Proc. R. Soc. London A 102, 161 (1922)], and tumbling. Interestingly, the order of modes is reversed for a prolate capsule: tumbling, precessing, and rolling with increasing dimensionless shear rate. At transitional regimes, we find the stable motion of a capsule can depend on its initial titled angle, even at the same shear rate. At high dimensionless shear rates, a spheroidal capsule undergoes a complicated oscillating-swinging motion: Its major axis oscillates about the plane

of shear in addition to the swinging about a mean angle with flow direction found previously, and the amplitudes of both oscillations decrease when increasing the dimensionless shear rate towards a steady tank treading motion asymptotically. The results are summarized in phase diagrams and the reorientations of both oblate and prolate capsules in a wide range of dimensionless shear rates are discussed.

P.05 Mechanical properties of keratin fibres in complex environments

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[1]Department of Chemistry and Centre for Scientific Computing, University of Warwick, UK, [2]Institute for Frontier Materials, Deakin University, Australia, [3]Unilever Research and Development, UK

Keratin fibres are an important structural component of cells, such as found in skin and nails, that form a cytoskeleton network which gives these cells an elastic response and flexibility.[1] Synthetic keratin films could inspire the development of novel biomaterials where flexibility or shock absorbance could be advantageous. The keratin fibre consists of a hierarchical assembly, starting with the lowest sub-unit; the keratin dimer.[2] While some macro-scale measurements are possible on keratin films and some in vivo fibres, it is very challenging experimentally to isolate and measure the physical properties of an intact dimer, without these denaturing or recombining into the full filament structure.

We have recently attained full atomistic structures of the K1/K10 keratin dimer[3] and are using these as a platform for gaining new insights into the mechanical properties of the fibre.[4] We have performed molecular dynamics simulations of the keratin dimer in its native solvent environment as found in skin – i.e. in the presence of natural moisturizing factors. By changing the environment we have investigated the impact on dimer mechanical properties. In an attempt to connect across the multiple lengthscales of this system and efficiently predict fibre properties, we have determined key energetic and mechanical parameters from the simulations and incorporated them into a mesoscale model of the keratin fibre.

[1] P. Strnad, V. Usachov, C. Debes, F. Gräter, D.A.D. Parry, M.B. Omary, Unique amino acid signatures that are evolutionarily conserved distinguish simple-type, epidermal and hair keratins*, Journal of Cell Science*, 2011, 124, 4221

[2] C.-H. Lee, M.-S. Kim, B.-M. Chung, D.J. Leahy, P.A. Coulombe Structural basis for heteromeric assembly and perinuclear organisation of keratin filaments*, Nature Structural and Molecular Biology*, 2012, 19, 707

[3] D.J. Bray, T.R. Walsh, M. Noro and R. Notman, Simulated full atomistic dimer structure of the epithelial keratin K1/K10 Intermediate filament, including the elusive head and tail domains, *in preparation*

[4] C-C Chou, MJ Buehler, Structure and Mechanical Properties of Human Trichocyte Keratin Intermediate Filament Protein, *Biomacromolecules*, 2012, 13, 3522

P.06 Ion channel gating by electrokinetic interactions

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Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK

Essential biological processes such as osmoregulation and transmission of nerve impulses crucially depend on translocation of water and ions through nanometre-sized membrane pores. In these processes, the electric fields, hydrodynamic interactions and osmotic gradients are inherently coupled, complicating theoretical analysis. Taking specific interactions between the channel surface and the ions into account, we solve the full set of electrokinetic equations in a geometry based on the crystal structure. We show that the gating kinetics of a simple model channel can be understood entirely in terms of electrostatic and hydrodynamic forces, together with membrane elasticity. The broad applicability of this approach makes it a promising candidate for future physical modelling of a wide range of gated ion channels.

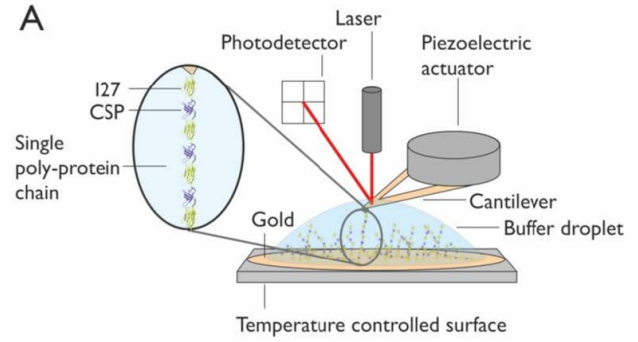
P.07 Variable temperature single molecule force spectroscopy of an extremophilic protein

K Tych[1,2], T Hoffmann[1,2], D J Brockwell[2] and L Dougan[1,2]

[1]Molecular and Nanoscale Physics Group, School of Physics and Astronomy, University of Leeds, UK, [2]Astbury Centre for Structural Molecular Biology and Institute of Molecular and Cellular Biology, University of Leeds, UK

Extremophiles (organisms which survive and thrive in the most extreme chemical and physical conditions on Earth) exhibit a range of fascinating cellular- and molecular-level adaptations [1]. The 'flexibility' of extremophilic proteins is one of the key determinants of their ability to function at the extremes of environmental temperatures [2].

We use single molecule force spectroscopy (SMFS) by atomic force microscopy (AFM) to measure the effect of temperature on the mechanical stability and flexibility of a protein derived from a hyperthermophilic organism, *Thermotoga maritima* [3]. Our chosen model protein is cold shock protein (CSP) B, a 66-residue nucleotide-binding protein with a known structure and with well-characterised thermodynamic and kinetic properties [4 - 6]. We construct a poly-protein chain consisting of CSP and I27, a marker protein, which provides a fingerprint for our studies [5].



Schematic illustrating the AFM SMFS variable temperature experimental setup – taken from [2]

The study was performed using an AFM SMFS instrument with variable temperature capabilities. In this experimental technique, a constant stretching force or a constant stretching velocity is applied along the end-to-end length of the protein, driving the protein into a fully extended unfolded state. We study temperature-dependent changes in the unfolding energy landscape of this protein by measuring changes in the unfolding force with temperature in combination with Monte Carlo simulations. We find that the position of the transition state to unfolding shifts away from the native state with increased temperature, reflecting a reduction in the spring constant of the protein and an increase in structural flexibility [2]. The mechanical robustness and malleability of this protein provides an insight into the dynamical properties of hyperthermophilic proteins.

[1] R.D. Macelroy, Biosystems 6: 57 – 80, 1974
[2] K. M. Tych, *et al.,* Soft Matter 9: 9016 – 9025, 2013
[3] T. Hoffmann, *et al.,* J. Phys. Chem. B 117: 1819 – 1826, 2013
[4] C. Motono, *et al.*, Proteins: Struct.,Funct.,Bioinf. 71: 655 – 669, 2008
[5] W. Kremer, *et al.*, Eur. J. Biochem. 268: 2527 – 2539, 2001
[6] C. Welker, *et al.*, Protein Sci. 8: 394 – 403, 1999

P.08 Modelling the transport of nanoparticles across the blood-brain barrier

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The blood-brain barrier (BBB) presents a physical barrier to the exchange of almost all molecules between the brain and the blood, restricting nearly all entry to the central nervous system (CNS) to via tightly regulated transport mechanisms. This presents a significant bottleneck in therapeutic intervention for neurological diseases, as >98% of small molecules and ~100% of large molecules are unable to access the brain tissue (Pardridge, 2005). Therefore, a coordinated strategy is required for the encapsulation and specific delivery of therapeutic molecules across the BBB. Recent interest has focused on the use of nanoparticles, functionalised to target natural transport mechanisms across the BBB, for delivery to the CNS. However, enhancing the properties of nanoparticles for optimal uptake requires rigorous testing of their physical and biological interactions. Furthermore, common *in vitro,* transwell models of the BBB, frequently used in the study of trans-BBB delivery, often demonstrate wide discord to *in vivo* models. We have constructed computational models of both *in vitro* transwells and *in vivo* capillaries. These models include considerations for nanoparticle behaviour under blood flow, particle-cell interactions and subsequent transport of particles. This permits the rapid screening of different nanoparticle compositions and moreover, helps explain disparity between *in vitro* and *in vivo* data.

[1] PARDRIDGE, W. M. 2005. The blood-brain barrier: bottleneck in brain drug development. *NeuroRx : the journal of the American Society for Experimental NeuroTherapeutics,* 2, 3-14

P.09 Folding of cellular monolayers

S Hoehn, P Haas, P K Trong and R Goldstein

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Cell sheet folding is a common morphogenetic process during the development of multicellular organisms [1]. Spheroidal green algae of the genus *Volvox* are uniquely suited as simple model systems for studying the basic principles of epithelial folding [2]. *Volvox* embryos turn their spherical cell monolayer inside out to achieve their adult configuration; this process is called inversion [2, 3, figure 1].

We use a combination of experimental and theoretical approaches to determine which cellular forces drive inversion and how these forces are forwarded across the cell sheet. Here we show comparative imaging of cell sheet folding in different *Volvox* species.

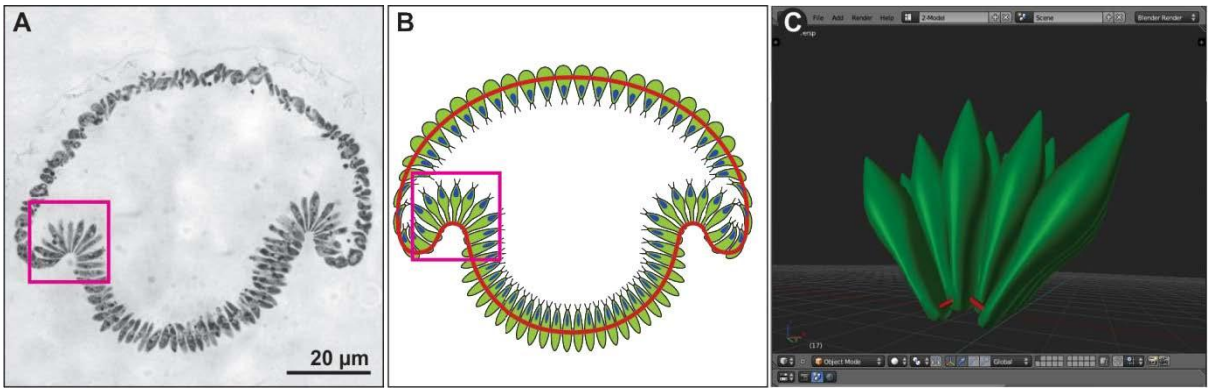

Figure 1. Inverting *Volvox globator* embryo. A: light micrograph. B: schematic representation. C: 3D-model of cells.

[1] Zartman JJ, Shvartsman SY: Unit operations of tissue development: epithelial folding. Annu Rev Chem Biomol 2010, 1:231-246
[2] Kirk DL, Nishii I: Volvox carteri as a model for studying the genetic and cytological control of morphogenesis. Dev Growth Differ 2001, 43:621-631
[3] Höhn S, Hallmann A: There is more than one way to turn a spherical cellular monolayer inside out: type B embryo inversion in Volvox globator. BMC Biology 2011, 9:89

P.10 Active polar fluid flow in deformable droplets

C A Whitfield[1], D Marenduzzo[2], R Voituriez[3,4] and R J Hawkins[1]

[1]Department of Physics and Astronomy, University of Sheffield, UK, [2]SUPA, School of Physics and Astronomy, University of Edinburgh, UK, [3]Laboratoire de Physique Théorique et Matière Condensée, UMR 7600, Université Pierre et Marie Curie/CNRS, France, [4]Laboratoire Jean Perrin, FRE 3231 CNRS /UPMC, France

At a continuum level, the eukaryotic cytoskeleton can be modelled as an active contractile fluid consisting of filaments and motors [1]. Here, we present some examples of analytical calculations of steady state flows of an active fluid confined to a circular/spherical droplet, that result from different internal configurations. We show that in some cases a droplet of active gel can be persistently motile when embedded in a suitable external medium. We compare these to simulations of the same system with a deformable droplet boundary, to observe how the droplet shape changes in its motile states. Therefore, this provides some simple quantitative examples of how cells can migrate in confinement (for example, embedded within a gel or tissue) and how the motility and deformation will depend on various physical parameters of the system.

[1] K. Kruse et al. Phys. Rev. Lett 92(7) 078101 (2004)

P.11 Is it possible the hydrodynamic synchronization of colloidal rotors describing rigid trajectories? - an experimental proof

A Maestro[1], N Bruot[1], J Kotar[1], N Uchida[2], R Golestanian[3] and P Cicuta[1]

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The coordinated cyclic beating of eukaryotic cilia and flagella is responsible for vital functions such as motility of microorganisms and fluid transport close to various epithelial tissues. Synchronization induced by hydrodynamic interactions is a possible and potentially general mechanism behind this coordinated beating of cilia. To understand hydrodynamic synchronization, rather than a realistic beating filament description, we use here a simple model with a minimal number of degrees of freedom, based on optically driven colloidal particles that can act as micron-scale phase oscillators. This model, known as “rotors”, has been studied recently by Uchida and Golestanian, who characterized the effective potential governing the dynamical states of a couple of rotors, predicting the stable and metastable states of the system by a theoretical analysis of the coupled-oscillator equation [1,2]. Building on our work of ref [3], we report here on a combination of experiments based on two colloidal rotors driven with optical tweezers along predefined trajectories and fixed force profiles. These experiments are backed by fully stochastic Brownian Dynamics simulations -including hydrodynamic interactions through the Blake tensor- to test the coupling potential that was predicted theoretically. In particular, we explore a wide range of physical conditions which lead to in-phase (or anti-phase) synchronization for an arbitrary trajectory shape.

[1] N. Uchida and R. Golestanian, Phys. Rev. Lett. 106, 058104, 2011
[2] N. Uchida and R. Golestanian, Eur. Phys. J. E. 35, 135, 2012
[3] J. Kotar, L. Debono, N. Bruot, S. Box, D. Phillips, S. Simpson, S. Hanna and P. Cicuta, Optimal hydrodynamic synchronization of colloidal rotors, Phys. Rev. Lett. 111, 228103, 2013

P.12 Short-time dynamics E. coli chromosomal loci reveal a dependence on coordinate and indicate the presence of a sporadic but ubiquitous super-diffusive motion

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University of Cambridge, UK

In recent years, evidence has emerged that the bacterial chromosome possesses a remarkable level of spatial and temporal organization, and its structural changes are believed to have an important role in key cellular functions, such as regulating transcription.

Particle tracking of chromosomal loci is possible by constructing strains in which GFP adheres to a particular genomic site. This has been used by several labs over the last few years both as a technique to map out the “home position” of each genomic site within the cell body, and to study the fluctuation properties. It has become a key technique in the development of a correct physical model to capture the in vivo structure and functional organization.

Our analysis of chromosomal dynamics investigated the short time (0.1s-10s) regime, published in [1], showing a decrease in motility in loci near the terminus of replication. This chromosomal trend is maintained across different growth conditions and appears to be related with the positioning of Ter in mid-cell position during chromosomal replication.

In unpublished work, we have compared the observed foci behavior with a physical model of subdiffusive dynamics, and we have found a small subset of ubiquitous “rapid movements” that exhibit near ballistic dynamics. This suggests the presence of an active driving machinery, or stress relaxation mechanisms that are non-trivially coupled with chromosomal partitioning; in either case, non-thermal fluctuations are present in the chromosome.

Finally, we have studied the effect on chromosomal dynamics induced by that chemical perturbations and in knockout mutants lacking certain nucleoid associated proteins.

[1] Javer, et al. "Short-time movement of E. coli chromosomal loci depends on coordinate and subcellular localization." Nature communications 4 (2013)

Colloids and nanoparticles

P.13 Design concepts for nanostructured colloidal composites

A Utgenannt[1,2], R Turner[1], A G Kanaras[2], O L Muskens[2] and J L Keddie[1]

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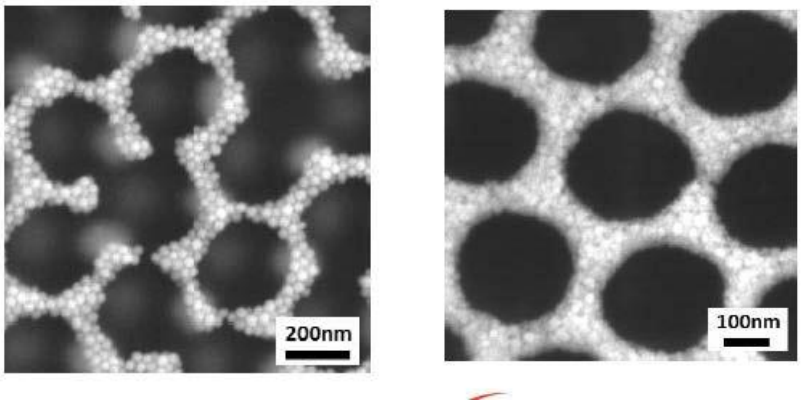
The assembly of colloidal nanoparticles into directed architectures is an emerging research theme that could enable the large-scale and low-cost fabrication of hierarchically structured nanomaterials, with applications in novel optoelectronic devices, sensors and metamaterials.[1-3] The self-assembly of nanoparticles can be employed as a low-cost approach compatible with large-scale device fabrication. However, the organization of plasmonic nanostructures over a large area (greater than several cm^2), achieved in a reliable self-assembly process, remains a grand challenge.[1,2]

Various types of fields (such as magnetic, electric or gravitational) can be used to guide and to direct the transport of colloidal particles. In this work, the transport of colloidal particles in water is directed in the vertical direction by variation of the balance between evaporation and diffusion. A Peclet number can be used to compare the rates of the two processes.[4] When diffusion is slow relative to evaporation (at a high Peclet number), particles accumulate near the top surface of a colloidal dispersion. In a binary blend of large and small particles, under the right

conditions, large particles are predicted to be concentrated at the top surface. However, a simple geometric argument reveals that when the large:small size ratio is greater than about 7:1, the smaller particles can be transported through the interstitial voids between the larger particles.[5]

In this work, we use a combination of microscopies and Rutherford backscattering spectrometry (for elemental depth profiling) to map out the nanostructures that are created over a broad range of evaporation rates and particle size ratios in binary blends of nanoparticles. Gold nanoparticles (10 nm and 30 nm diameters) are blended with hard polymer particles with sizes ranging from 100 to 400 nm.[6] The evaporation rates are controlled by varying the water temperature (with infrared heating) and the relative humidity. The polymer particles sinter under IR radiative heating so that a hard nanocomposite coating results. We show that an understanding of the fundamental mechanism can be used to design various types of nano-ring structures, such as those shown here, along with more random structures, depending on the processing conditions and particle size ratios.



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P.14 Nucleation of hard colloidal cubes

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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 emergence 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.

Unlike hard spheres, the simple cubic crystal lattice of hard cubes exhibits a reasonable amount of vacancies near coexistence. Smallenburg et al. [2] showed that this finite vacancy concentration in fact stabilizes the crystal and by doing so, lowers the melting point. In addition to the high vacancy concentration, the crystal is characterized by relatively fast diffusion near coexistence. Hence, coming from the liquid phase, hard cubes will nucleate into this dynamic, vacancy rich crystal.

In this poster we will present the dynamics of the freezing transition of hard colloidal cubes. To study the properties of the transition we used kinetic Monte Carlo, combined with rare event sampling techniques such as Transition Interface Sampling.

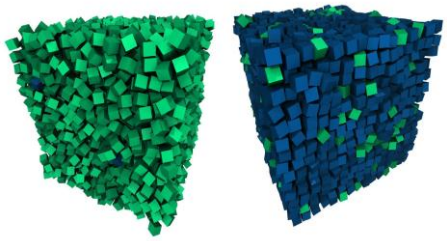

Figure 1: Cubes at packing fractions ϕ = 0.44 close to freezing point (left) and ϕ = 0.52 close to melting point (right). The cubes are colored according to the value of an order parameter that measures the relative orientations, blue denoting cubically ordered and green denoting unordered.

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P.15 The reciprocal theorem for two objects

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The reciprocal theorem for Stokes flows has become a standard tool in the study of the motion of objects in a viscous fluid with no net forces, such as swimming microorganisms or artificial self-propelled particles. Here we present an extension of this principle to study the pairwise interactions of such objects with each other in three simple cases, using complex variable techniques: a) diffusiophoretic interaction of an isotropic spherical source with a fixed or free inert object; b) a pair of simple Janus-like spherical swimmers; and c) a pair of treadmilling swimmers with dipolar flow fields. We find hydrodynamically bound chains of simple swimmers, and a quasi-stable configuration of treadmillers reminiscent of the celebrated 'waltzing' of Volvox colonies.

P.16 PNIPAM microgels: A novel insight into their adsorption at fluid interfaces

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The thermo-responsive character of Poly N-Isopropyl Acrylamide (PNIPAM) microgels plays a key role in their affinity for fluid interfaces by tuning their adsorption ability. Further, the confinement of PNIPAM particles to a two-dimensional scenario gives rise to their conformational change causing them to spread out at the interface, along with an in-plane spatial re-organization.

We address here the effect of the temperature on the confinement of PNIPAM particles to a two-dimensional scenario such as the decane/water interface. These microgel particles are adsorbed irreversibly creating fluid-like layers at the interface. A jamming transition is observed when the accessible interfacial area is reduced. We note how the fluid-to-solid transition occurs at progressively lower area fractions as the temperature increases. By varying the temperature and hence the size and softness of the particles, we demonstrate which are the key factors controlling this jamming transition.

[1] Omkar S. Deshmukh , Armando Maestro, Michel Duits, Dirk vanden Ende, Martien Cohen-Stuart and Frieder Mugele*; to be submitted.*

P.17 Unusual order in squeezed spheres

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This contribution deals with the arisal of structures with an unusual symmetry from purely repulsive isotropic pair potentials. The most obvious of such potentials, such as power laws and gaussian core potentials, give energy minima that are triangular close packed structures in 2D and FCC or BCC in 3D.

It turns out that the soft spheres that the jamming community has been using for years to study disordered solids near the jamming transition, give rise to a range of surprising ordered structures at higher densities, as has already been reported for Hertzian disks [1], and for harmonic and Hertzian spheres in three dimensions [2, 3, 4],. Monodisperse repulsive harmonic disks in two dimensions form, apart from the triangular lattice everyone would expect, a square lattice and various non-bravais lattices that can be related to tiny periodic packings of hard spheres. These include the honeycomb, a stretched honeycomb, a chiral structure, and a previously unreported lattice that has a 5-particle basis. The essential physics behind the appearance of these structures amounts to a trade-off between “having one’s nearest neighbours further away” and “having fewer nearest neighbours”.

These findings allow us to make a few key observations about the ways systems of repulsive particles can respond to changes in density, including the possibilities to compress anisotropically, to deform non-affinely, and to transition to a different symmetry via a coexistence region. All of these options are realized by harmonic disks in 2D. A rough sketch of the resulting phases is shown in figure 1. Although it is unlikely that this particular potential, at these higher densities, represents a realizable physical system, there may well be other potentials with similarly rich behaviour. Preliminary studies of a recently introduced effective potential for adsorbed star polymers are promising in this respect [5].

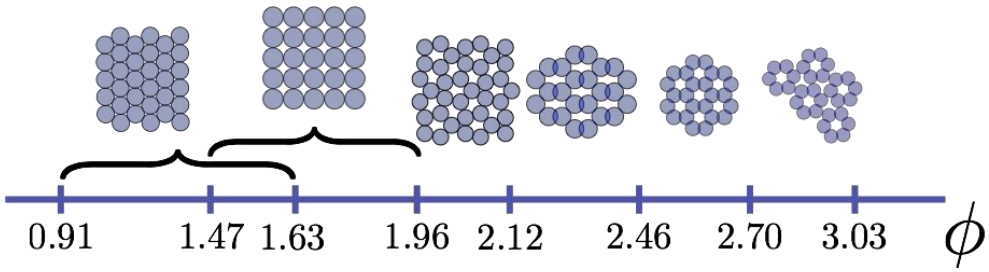

Figure 1: Sketch of $T = 0$ phases diagram of harmonic disks (drawn smaller for clarity) in 2D, as a function of “area fraction”. The nature of the transitions will be discussed in the talk.

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P.18 Deposition of colloidal asphaltene in capillary flow from computer simulation and homogeneous deposition models

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We have investigated the deposition of colloidal particles, such as crude oil asphaltenes, in capillary flow as a function of increasing flow rate using the hybrid Stochastic Rotation Dynamics – Molecular Dynamics approach. The simulation results are compared with experimental results and homogeneous deposition models. First, we derive expressions for the deposit thickness $e(t)$ for both constant flow rate (as in the experiment) and constant pressure drop (as in the simulations). We investigate the accuracy of expressions, based on the assumption of Poiseuille flow, to estimate the deposit thickness from pressure drop or flow rate measurements. Our conclusions are twofold. First, for low flow rates ($Pe \leq 10$ for our system), we observe that the dimensionless deposit thickness $e(t) / r(0)$ as estimated from the flow rate is in good agreement with direct fractional deposition measurements. This implies that the homogeneous deposition approximation works well at low flow rates. Second, for higher flow rates ($Pe > 10$ for our system), we observe that the difference between the estimated deposit thickness and the actual deposition thickness increases with increasing flow rate. This suggests that the homogeneous deposition approximation is no longer valid at high flow rates. Detailed calculations of the flow field confirm that, at high flow rates, large clusters of colloids are flowing through the capillaries and generate transient plug flow, disturbing the laminar flow field. Therefore care must be taken when estimating the dimensionless deposit thickness from flow rate or pressure drop measurements.

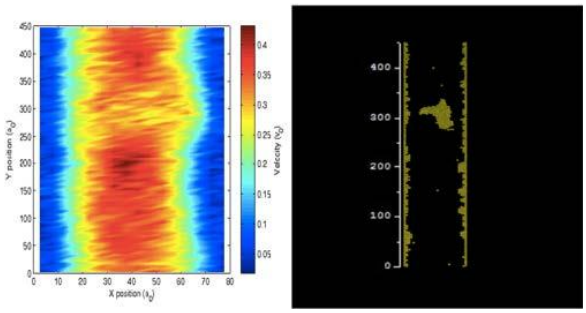

Figure 1: Flow field showing the solvent velocity magnitude across the capillary with corresponding snapshot of the capillary. As can be seen there is a distortion in the flow field present at the position of the large cluster in the capillary.

Confined fluids and interfacial phenomena

P.19 Predicting anomalous fluid densities in carbon nanotubes

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The equilibrium density of fluids under nanoconfinement can differ substantially from their density in the bulk [1]. Understanding the physical basis for and magnitude of these anomalous densities is important for a broad range of nanoengineering applications, such as the design of nanoporous desalinators or the extraction and storage of fluids in nanoporous media. We present here the results of molecular dynamics simulations conducted in LAMMPS that study the equilibrium densities of a hard-sphere Lennard-Jones fluid and water confined within carbon nanotubes (CNTs). We observe that both fluids exhibit decreasing densities under increasing confinement due to repulsive fluid-CNT interactions, in agreement with the literature [2][3]. We find that *within* either fluid's maximum

energetically accessible radius, the fluid density is actually *greater* than the bulk density. Finally, we present an analytical model that accurately predicts the maximum energetically accessible radius. We will also discuss the prospects for predicting anomalous fluid densities in the extreme case of single-file confinement using an Ising-like model.

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P.20 Direct effects of non-equilibrium aggregates on Pdadmac/SDS layers at the air/water interface

R A Campbell[1], M Yanez Arteta[1,2], T Nylander[2], B A Noskov[3] and I Varga[4]

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The exploitation of non-equilibrium effects in oppositely charged polyelectrolyte/surfactant (P/S) mixtures is attracting more and more attention.[1–3] Here we discuss various different mechanisms to explain the non-equilibrium properties of P/S mixtures at the air/water interface in terms of adsorption vs. trapping or spreading of particles delivered by convection[4] vs. deposition under gravity.[5] Poly(diallyldimethylammonium chloride)/sodium dodecyl sulfate (Pdadmac/SDS) samples have been examined with respect to the bulk composition, changes in the bulk phase behavior and sample history using ellipsometry, neutron reflectometry and Brewster angle microscopy (BAM). Aggregate penetration into the adsorption layer is observed from kinetically-trapped particles at the edge of the phase separation region for *fresh-mixed* samples. For the supernatant of well-equilibrated *aged- settled* samples, penetration of aggregates occurs only when the particles are positively charged, which is attributed to their interaction with the negatively charged headgroups of the surfactant monolayer. Through the application of a light mechanical stress to the sediment, the surface properties of *aged-redispersed* samples are significantly modified, and the change in the interfacial properties is again faster for samples with positively charged aggregates. Trapping of particles at the interface occurs for samples where the surface is not subjected to cleaning by aspiration, and the process is most prevalent at compositions close to charge neutralization (0.82 mM; see figure). This work begins to outline the complexity of how non- equilibrium P/S aggregates can dramatically impact the interfacial properties directly. The implications of our findings are discussed in terms of material applications.

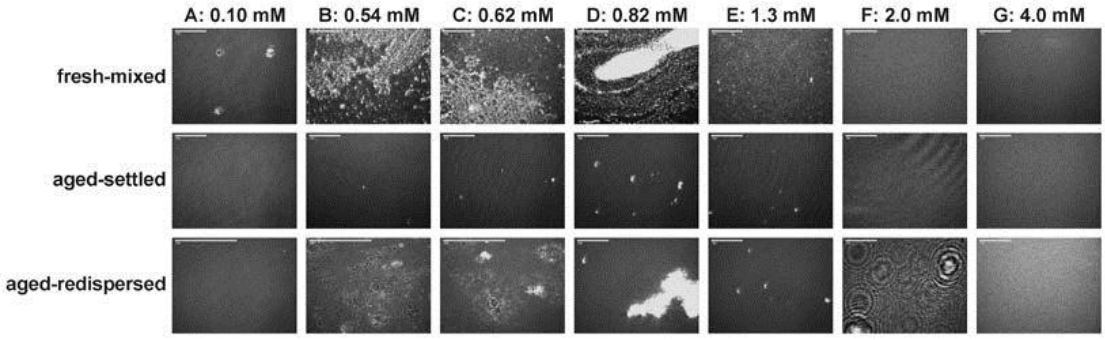

Figure. BAM images of *fresh–mixed*, *aged–settled* and *aged–redispersed* 100 ppm Pdadmac/SDS samples in 0.1 M NaCl without surface cleaning by aspiration. The scale bars are all 100 µm.

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P.21 A Landau-Squire nanojet

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Fluid jets are found in nature at all length scales, from microscopic to cosmological. We have been investigating what may be one of the smallest liquid jets ever observed: an electroosmotically driven flow from a single glass nanopore about 75 nm in radius with a maximum flow rate around 30 pL/s. A novel anemometry technique allows us to map out the vorticity and velocity fields which show excellent agreement with the classical Landau-Squire solution of the Navier Stokes equations for a point jet. We observe a phenomenon that we call flow rectification: an asymmetry in the flow rate with respect to voltage reversal. In addition to technological applications in nano patterning and microfluidics, such nanojets are fascinating because their behaviour is intricately linked to the mechanisms of ion transport and rectification in biological and artificial nanopores.

P.22 Hindered diffusion coefficients of spherical particles confined by microchannels

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We present here the measurement of the diffusivity of spherical particles closely confined by narrow microchannels. Our experiments yield a 2D map of the position-dependent diffusion coefficients parallel and perpendicular to the channel axis with a resolution of down to 129 nm. The diffusivity was measured simultaneously in the channel interior, the bulk reservoirs as well as the channel entrance region. In the channel interior we found strongly anisotropic diffusion. While the perpendicular diffusion coefficient decreased with the distance to the confining walls down to approximately 25% of the value on the channel axis, the parallel diffusion coefficient remained constant throughout the entire channel width. In addition to the experiment, we performed finite element simulations for the diffusivity in the channel interior and found good agreement with the measurements. Our results reveal the distinctive influence of strong confinement on Brownian motion which is of significance to microfluidics as well as quantitative models of facilitated membrane transport.

Liquid crystals / Liquids and glasses

P.23 Crystallization mechanism in melts of short n-alkane chains

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Despite the long-standing research interest in crystallization in polymer melts, many fundamental aspects of the crystal nucleation and growth mechanisms are still subject of discussion [1, 2].

Experiments in this field are usually restricted to a spatial and temporal resolution that is too coarse to capture atomistic details of individual nucleation events. Thus molecular dynamics provides an ideal instrument to complement experiment and offer insight into the mechanisms on the atomistic scale.

In the traditional picture of the early stages of the polymer crystallization, the Bragg peaks are observed after the induction period in wide angle X-ray scatter- ing(WAXS). No small angle X-ray scattering (SAXS) peak is expected before the Bragg peak. But in 1990's SAXS peaks were reported in many experiments during induction period before the appearance of the Bragg peaks [3, 4, 5]. These SAXS peaks were claimed to be due to the presence of ordered melt before occurrence of nucleation event. Theories have been proposed to explain these SAXS peak [6, 7].

Given the high degree of complexity that long polymer chains pose both, from the conceptual and the numerical point of view (due to folding and entanglement), a basic comprehension of how even relatively short chains crystallize is of fundamental importance in order to build a coherent theory.

Crystal nucleation in alkanes has been addressed in several computer simulation studies in the 90s [8, 9, 10, 11] and a scenario for the nucleation mechanism has been suggested. Due to the limited computer resources available at the time, however, these works were based on one simulation trajectory each (with the exception of ref. [8]).

Considering the limited amount of data available in the literature on the nucleation and growth mechanism in short chain alkanes, we have revisited the problem and present here a detailed analysis of the formation of crystal nuclei from the homogeneous melt and the subsequent growth process.

We study crystallization in a model system for eicosane (C20) by means of molecular dynamics simulation and we identify the microscopic mechanisms of homogeneous crystal nucleation and growth. For the nucleation process, we observe that chains first align and then straighten. Then the local density increases and finally the monomer units become ordered positionally. The subsequent crystal growth process is characterized by a *sliding-in* motion of the chains. Chains prefer- ably attach to the crystalline cluster with one end and then move along the stems of already crystallized chains towards their final position. This process is cooperative, i.e. neighboring chains tend to get attached in clusters rather than independently.

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P.24 Effect of temperature on orientational ordering in a modified Gay-Berne fluid

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A second order density-functional theory has been used to study the effect of varying temperature on the orientational ordering in a fluid of molecules interacting via a modified Gay-Berne potential in which the attraction force can be tuned by adjusting one parameter only. An attractive parameter Ps has been introduced in the Gay-Berne potential for describing the strength of attractive force relative to its repulsive counterpart. The direct pair-correlation functions of the isotropic phase that enters in the density-functional theory as input information have been obtained by solving the Ornstein-Zernike equation using the Percus-Yevick integral equation theory for different densities, (reduced) temperatures and attractive parameters. The isotropic-nematic phase coexistence and thermodynamic parameters of liquid crystal have been investigated using density-functional theory. The theoretical results have been compared with the available computer simulation results and the traditional Gay-Berne potential.

P.25 Electron transitions in Cr^{2+} in the aqueous solutions of $MgSO_3.6H_2O$:Cr

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The cations of 3d metals in water and alcohol create aqueous complexes. The creation and stability of the aqua cations are important. The number of water molecules which are connected with the metal by the direct bonds metal-oxygen determines the properties of the complex. The classical investigations, for example: mobility of the ions, ostensible radii of the hydration ions and the entropy of hydration do not give detailed information for the aqua ions. This is the reason for the investigation of their spectral properties. These properties depend on the composition and the symmetry of the surrounding medium.

In this work, the absorption of the complex $[Cr(H_2O)_6]^{2+}$ is measured in the spectral region 375 – 700 nm. The aqueous solutions of $MgSO_3.6H_2O$:Cr are prepared with the concentrations 0.4%, 0.6% and 0.8%. The energies of the electron transitions in Cr^{2+} are calculated. The role of the spin-orbit coupling Hamiltonian is evaluated also. Zeeman splitting which is characteristic for Cr^{2+} is determined and discussed.

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Polymers, polyelectrolytes and biomolecules

P.26 Cross-sectional imaging of organic solar cells: Understanding efficiency and lifetime issues

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Organic solar cells offer a potentially cheaper alternative to traditional solar technologies, but presently have low efficiencies and poor lifetimes. The structure of the cell and the morphology of the polymer blend forming the active layer are important in attempts to achieve higher efficiencies, whilst not much is presently known about causes of failure and degradation pathways.

TEM imaging of FIB cross-sections allows such devices to be viewed, both before and after cells have been used – offering advantages over other techniques such as AFM which only examine the surface. This approach has enabled us to study the active layer and also the electrical contact layers in real devices. Phase separation in the active layer has previously been observed by TEM [1] but similar results have not been seen here. The similar atomic composition and densities of the two materials means that very little contrast is observed with TEM. This is made more challenging by the miscibility of PCBM [2], the averaging effect of viewing through a three-dimensional sample and the difficulties in accurately interpreting defocused TEM images [3].

This cross-sectional imaging has also been used to study degradation. Water and oxygen are known causes [4] and by observing what is happening in the cell at various stages in the degradation process, failure mechanisms can be better understood. By exposing cells to high humidity it has been shown that the grain size of the aluminium used in the cathode changes the extent of the degradation observed. The use of calcium in the cathode and choice of material for the hole transport layer also affect the degradation. This knowledge should enable cell design to be improved to increase device lifetime.

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P.27 Computational studies on the effect of stereotacticity of poly(N-isopropylacrylamide) in aqueous solution

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Lehrstuhl für Technische Thermodynamik, RWTH University, Germany

In the present work the effect of polymer tacticity on the solubility and the lower critical solution temperature (LCST) of poly(N-isopropylacrylamide) (PNIPAM) chains in water is investigated by means of molecular dynamics simulations. The extent and type of stereoregularity of the polymer chains have a significant impact on the LCST of PNIPAM in aqueous solutions: the transition temperature, above which a polymer chain exhibits an abrupt and reversible coil-to-globule transition, is considerably reduced for the isotactic-rich polymers and scarcely increased for the syndiotacticrich polymers compared to atactic polymers. Previous computational studies on the deswelling mechanism of stereoregular NIPAM-oligomers in water and water-alcohol mixtures, though indicating conformational

entropy change associated with different stereoisomers, were all limited to dimers and trimers. It was shown, however, that in simulations a distinguishable coil-to-globule transition in a single polymer chain appears first with a chain length of at least 30 monomer units.

To investigate the effect of stereotacticity on the hydration of PNIPAM polymers atomistic molecular dynamics simulations of a single NIPAM-oligormer consisting of 30 monomer units solvated in water are used to model two limiting cases of iso- and syndiotactic isomers below and above LCST. The deswelling of PNIPAM chain is clearly observed at different temperatures for different stereoisomers. Conformational transitions in these two stereoisomers are evaluated using structural and dynamical correlation functions such as radius of gyration, pair correlation function, spatial distribution functions of water molecules and auto-correlation functions of intra- and intermolecular hydrogen bonds. Our results suggest that stereoisomers have different steric volume that greatly affects the conformational transition of chains and different LCST temperatures. The carbonyl oxygens located on the same side of the backbone of an isotactic PNIPAM chain hinders the formation of H-bonds between solvent and polymer to some extent and this effect should be also present in similar thermosensitive polymers, e.g. poly(N,N-diethylacrylamide). In addition, we calculate the radial and spatial distribution of water molecules around isotactic and syndiotactic solutes and indicate the difference in this distribution is mainly due to the steric effects. Thus, our study provides atomic-scale insights into the role of stereotacticity in deswelling transition of PNIPAM across LCST.

P.28 MD and COSMO-RS contact statistics for poly(N-isopropylacrylamide) in solvents

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The relatively new class of gels, the so-called microgels are chemically inert systems, which are responsive to changes of the environment by changing their shape and size. Therefore, an enormous potential in the area of drug delivery is attributed to microgels.

A phenomenon, which is not fully understood and still under debate in the literature, is the so-called cononsolvency effect. Thereby it can be observed that even if a particle is swollen in two pure solvents, it is collapsed in a mixture of the two solvents.

Molecular dynamics (MD) simulations were carried out to investigate the volume phase transition behaviour poly(N-isopropylacrylamide) (PNIPAM) polymer at the atomic level. Polymer chains consisting of 3 to 30 monomers units were solvated in water, methanol and water-methanol mixtures of different concentrations and/or different temperature below and above the lower critical solution temperature.

The COSMO-RS (Conductor-like Screening Model for Real Solvents) model allows for the predictive calculation of chemical potentials in almost arbitrary mixtures. It consists of a DFT (Density Functional Theory) calculation of each molecule in a virtual conductor, yielding the surface screening charge density distribution. Based on this, the interaction energies of molecules in contact are computed and thereby the chemical potential of each species are available. Therefore any thermodynamic data is available, including the phase transition behaviour.

As the surface contacts in the COSMO-RS model define all interaction properties, we analysed the MD trajectories for the purpose of molecular contact statistics by applying Voronoi tessellations to the configurations of the swollen and deswollen states of PNIPAM. The obtained results were compared with the COSMO-RS contact statistics. We expect that the analysing methodologies can be extended to other polymeric hydrogels and solvents, which will contribute to understand the observed phenomena and developing new polymer hydrogels with finely tuned characteristics.

P.29 Transition path sampling with core-modification aimless shooting for a homopolymer chain

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We investigate the crystallization of a single, flexible homopolymer chain [1,2] using transition path sampling (TPS) [3] with a new shooting move tailored for simple polymers [4]. The chain consists of *N* identical spherical monomers evolving according to Langevin dynamics. While neighboring monomers are coupled via harmonic springs, the non-neighboring monomers interact via a differentiable approximation to a square-well potential. In our study, we verify the similarities between a pure square-well chain with fixed distances and our continuous approximation. For a sufficiently small interaction range λ, the system undergoes a first-order freezing transition from an expanded, unordered phase to a compact crystalline state. TPS and committor analysis [5] are used to study the transition state ensemble of the *N*=128 chain and to search for possible reaction coordinates based on likelihood maximization methods [6]. Earlier observations concerning the structural properties of the transition states for the pure square-well chain are are also seen in our simulations: The typical transition states consist of a crystalline nucleus attached to one or more chain fragments. Furthermore, we show that the new core-modification shooting move strongly increases the sampling efficiency of the TPS simulation.

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[5] Elisabeth Scholl-Paschinger and Christoph Dellago, "Demixing of a binary symmetric mixture studied with transition path sampling", Journal of Chemical Physics 133, 104505 (2010)
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P.30 Self-assembly of degalatosylated xyloglucan from tamarind seeds

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Xyloglucans are cellulose-like natural polysaccharides having a molecular structure highly branched and rich of hydroxyl groups. Xyloglucan extracted from tamarind seed has β(1,4)-D-glucan backbone, the same as cellulose, partly substituted by α(1-6)-D-xylopyranosyl side chains, some of which are further substituted by β(1,2)-D-galactopyranosyl residue.

In its native form the biopolymer is quite soluble in water and forms gel only in presence of alcohols or sucrose. When a given fraction of galactosyl residues are removed by enzymatic reaction, the polymer becomes able to form thermo-reversible hydrogels in pure water at physiological temperatures. Due to the relevance of this property for biomedical/pharmaceutical applications, a large interest is emerging about this system and the way to control or manipulate its aggregation/gelation propensity.

In this work we study the effects of the temperature on the conformation and organization of degalactosylated xyloglucan chains in aqueous solution at concentration low enough not to run in macroscopic gelation. In fact, our aim is to figure out at molecular level the mechanism by which the tuning of hydrophobic interactions leads to self-assembly and/or macroscopic gelation. The polymer solution at 0.1% w/w concentration was investigated at 15 and 37 ^{0}C by different experimental techniques (Static and Dynamic Light Scattering, Small Angle X-ray Scattering,

Rheology, Circular Dichroism). The fluorescent probe 1-anilinonaphthalene-8-sulphonic acid (1,8-ANS) was used to assess the change of exposed hydrophobic surface due to the self-assembly of the polymer.

Results show that, on increasing temperature, the polymer chains and pre-existing clusters form larger structures, but the aggregation is accompanied by a density increase occurring on small length scale and similar to that observed in formation of dendrimeric structures. The relation of these results to coil-globule transition and phase separation is discussed.

P.31 Key factors regulating the mass delivery of macromolecules to model cell membranes: gravity and electrostatics

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An immense research effort has been invested to understand the mechanisms of interactions between macromolecules and cell membranes.[1] Positively charged macromolecules can be recruited into the cell by the endocytosis pathway and then trafficked by different organelles according to their charge.[2] A key challenge is to develop drug delivery systems involving the efficient transport of therapeutic agents to lipid membranes.[3] One approach is to position reservoirs of the drug in contact with the membrane for continuous delivery by slow diffusion.[4] In this case the drug may be encapsulated into aggregates of lyotropic phase,[5] providing a way to reduce dosages and the frequency of injections administered to patients.

Here we show that both gravity and electrostatics are key factors regulating interactions between model cell membranes and self-assembled lamellar aggregates of dendrimers and phospholipids. The system is a proxy for the trafficking of reservoirs of therapeutic drugs to cell membranes for slow diffusion. Neutron reflectometry measurements were carried out on supported lipid bilayers of varying charge and on hydrophilic silica surfaces. Using a novel approach, we made measurements both above and below the bulk liquid to highlight effects of bulk phase separation and gravity on the interfacial properties. Translocation of the macromolecule across the membrane and adsorption of the lamellar aggregates occur only when the membrane (1) is located above the bulk liquid and (2) has sufficient negative charge. The directionality effects were dramatic and we seek to emphasize their effects to researchers involved in biochemical investigations of complex formulations in the future. Further, our findings indicate the potential to switch on the interaction mechanism through tuning the charge of the aggregates to activate endocytosis pathways on specific cell types, which we discuss in the context of future targeted drug delivery applications.

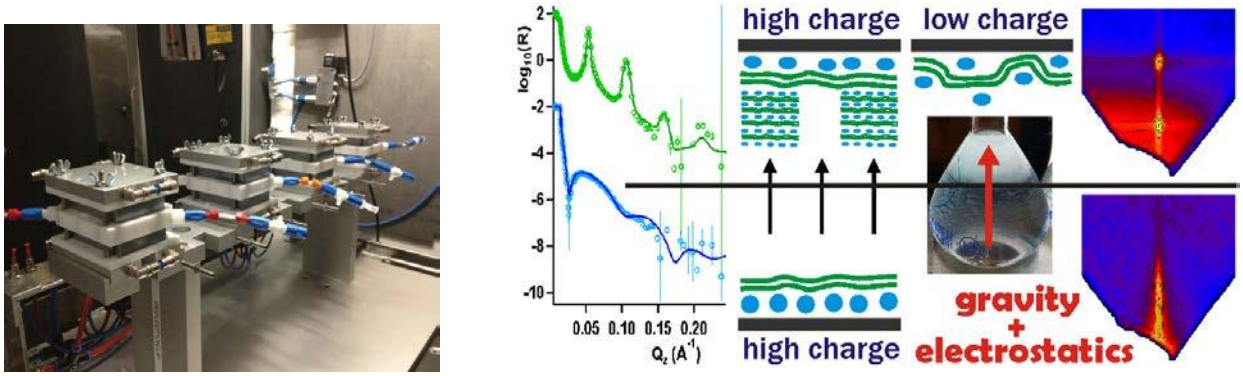

Figure. Left. The unique solid/liquid/solid interface designed specifically for this study. Right. Table-of-contents image from our publication in *ACS Macros Letters* from January 2014.[6]

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P.32 Hydration dynamics of proteins in solutions studied in 220-325 GHz band

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The transmission measurements of protein water solutions have been performed using a vector network analyser-driven quasi-optical bench covering the waveguide band 220-325 GHz. The following proteins, ranging from lower to higher molecular weight, were chosen for this study: lysozyme, myoglobin and bovine serum albumin (BSA). A special liquid cell with TPX windows and 100 μm window separation (spacer) have been used to study these. Defined amounts of each protein were dissolved in distilled water without adding any salt-buffer. Absorption properties of solutions were studied at different concentrations ranging from 2 to 100 mg/ml. The molecular dynamics simulator Gromacs was used to accurately estimate the number of water molecules excluded by each protein. The initial purpose is to check whether all protein solutions consistently exhibit a decreased absorption compared to bulk water (THz defect) in the lower THz spectral domain (0.22 – 0.325 THz). A THz defect was the expected scenario, since protein molecules have far less absorption than water molecules. However at low protein concentration the recorded spectra showed an initial rise or a plateau in absorption compared to bulk water (THz excess) followed by a decrease in absorption. This non-linear trend in solution absorption was consistently observed for all three proteins. According to our findings, this point of inflection is not related to the onset of the protein hydration shells overlap, since it occurs at rather dilute concentrations. Instead, the results suggest that the molar protein absorption in solution is significantly higher compared dry-state protein. This effect is especially evident at low protein concentrations of about 10-20 mg/ml. Previously THz excess of protein solutions has been reported only at frequencies above 2 THz. The data obtained shows that three different protein solutions consistently exhibit THz excess in the lower THz domain considered. This in turn suggests that protein water interaction is more complex than previously believed.

P.33 Nanostructuring thin polymer films with 2 and 3-beam single pulse laser interference lithography

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Laser ablation is one of the most used approaches to fabricate micro and nanostructures. Nevertheless, writing more than one of these features at a time requires the use of a mask. Laser Interference Lithography (LIL) allows overcoming this limitation and writing a whole array of structures at once.[1] The application of these patterning technique to polymer thin films has been scarcely reported in the literature,[2] and the use of 3-beam LIL in polymeric materials has not been reported to our knowledge. In this work, 2 and 3-beam Single Pulse Laser Interference Lithography has been applied to thin polymer films obtaining micro and nanogratings as well as nanocavities arranged in a distorted hexagonal lattice. The formation mechanism of ablation in polymer thin films has been studied by inspecting different regions of the sample corresponding to different laser fluences. The assessment of the resulting structures has been carried out in real (AFM) and reciprocal (GISAXS) space, showing the solid structural order of the samples and the well defined morphology of the structures.

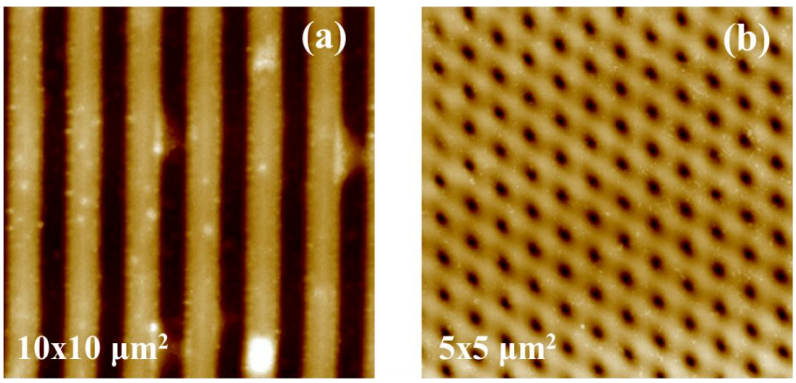

Figure 1. AFM topography maps of structures fabricated in thin polymer films by LIL: (a) microgratings fabricated by 2-beam LIL and (b) nanocavities fabricated by 3-beam LIL.

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Rheology and non-equilibrium phenomena

P.34 Active nematic dynamics in a viscoelastic background

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The term active soft matter describes a fascinating class of materials that are kept out of thermodynamic equilibrium by an internal energy source, normally in a biological context [1]. We present some initial analytical and numerical results from a novel model [2] ideally suited for studying the hydrodynamics of an active gel (such as actomyosin, found in the cell cytoskeleton) which couples active liquid crystal dynamics to a polymeric background. This coupling can lead to exotic rheological properties that strongly effect phenomena such as shear banding and zero Reynolds number “bacterial turbulence”: these form just a small part of a rich and varied phase diagram.

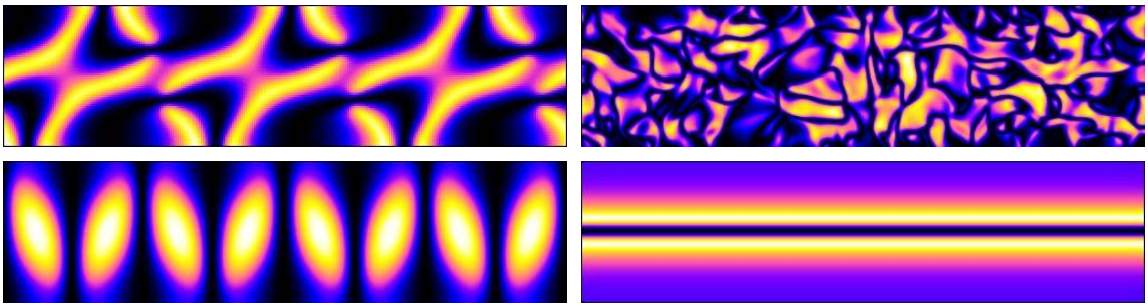

Figure 1: Example of some of the states found in the phase diagram (shown is $n_x n_y$ where $\hat{\boldsymbol{n}}$ is the liquid crystal director).

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P.35 Simulation of the linear and non-linear rheology of viscoelastic polymer solutions

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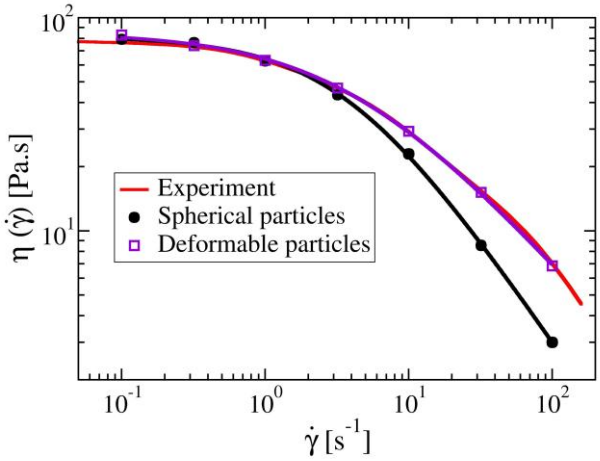
The use of coarse-grained approaches for the simulation of polymer liquids allows access to substantially larger time and length scales that are impossible to reach through atomistic simulations. Coarse graining of any polymer system simplifies both the polymer representation and the description of toplogical constraints or inter---polymer entanglements. Various degrees of coarse-graining are possible such as representing a group of monomers as a blob or bead to a highly coarse-grained view where each entity is described as a point particle.

We present simulation results of the linear and non-linear rheology of two viscoelastic polymer solutions using a highly coarse-grained approach known as the Responsive Particle Dynamics (RaPiD) model. RaPiD, which is a mesoscopic model based upon Brownian dynamics, has been successfully employed for the simulation of shear banding, particle alignment and chain diffusion in viscoelastic fluids [1]. In RaPiD each constituent polymer has until now been viewed as a spherical particle with the effects of the eliminated degrees of freedom included through the selection of an appropriate free energy and transient pair-wise force. Here we update the particle description to account for particle deformability by allowing all RaPiD particles to elongate. The inclusion of this particle deformation is shown to be crucial towards recovering the experimental non-linear rheology i.e. shear thinning effects, for both polymer solutions. We also preserve the description of the linear rheology with the update to the deformable particle representation [2].



Demonstration of the recovery of the non-linear rheology of a polymer solution using the RaPiD deformable particle model.

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P.36 Plastic deformation mechanisms in glassy and semi-crystalline polymers

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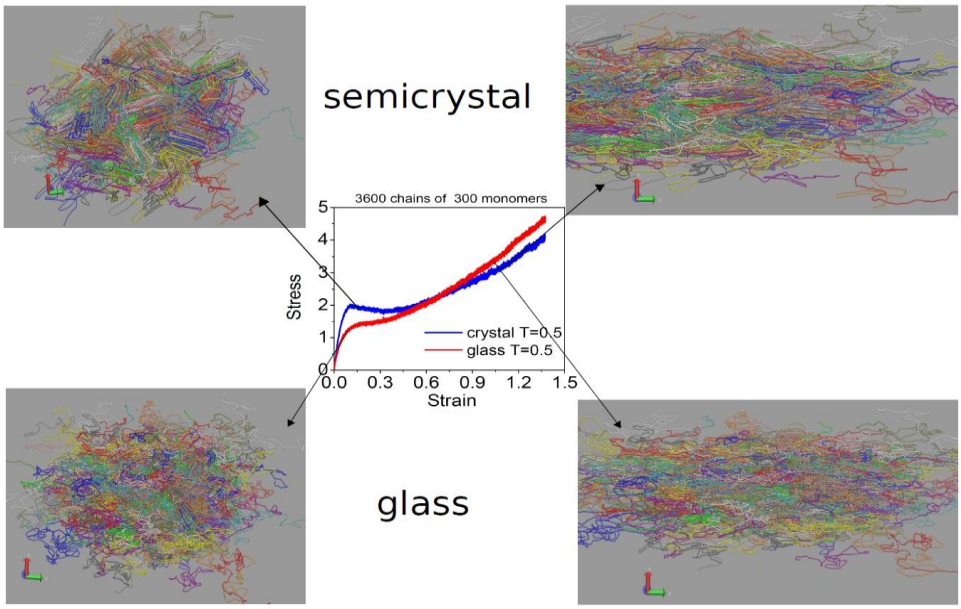
In polymeric materials, the connectivity of the long chain molecules usually hinders the formation of perfect crystals. However, upon slow enough cooling, polymers with regular side chains form partially crystalline structures that consist of stacking chain folded lamella and amorphous regions. The interplay of crystalline and amorphous regions leads to non-brittle solid materials with increased toughness that makes them favorable for various industrial applications. Although there is a wide agreement on the structure of this semicrystalline phase [1] mechanisms of deformation under stress, particularly at single chain level, are poorly understood and a subject of debate.

In order to gain an insight into the mechanical response of semi-crystalline and glassy polymers, we use molecular dynamics simulations. We employ a coarse-grained model for semiflexible polymers (CG-PVA) [2] which displays both crystallization and glassy behaviour via changing the cooling rate. We investigate the mechanical response of polymers by means of uniaxial tensile tests [3]. We address two key questions: i) How do ordered and amorphous regions transform under uniaxial tension? ii) How do mechanical properties of semicrystalline polymers differ from glassy ones?



We obtain the stress-strain curves in both elastic and plastic regimes of deformation and analyze the configurations of deformed samples (see figure). For semi-crystalline samples, in the elastic (linear) regime, deformation leads to a slight stretching of amorphous chains. Upon further increase of strain and yielding of samples, we observe a partial loss of crystallinity accompanied by partial alignment of crystallites with the tensile direction. Very large deformations cause unfolding of lamella and further stretching and alignment of chains along the tensile direction. In glassy samples, small deformations leads to stretching of chains and further increase of tension leads to a greater extent stretching and alignment of chains with tensile direction.

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P.37 Dynamics and structure: a study of gelation in a non-aqueous colloidal system

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Overbased detergents are a class of engine oil additive, comprising a metal carbonate core (typically 1-10 nm in diameter) surrounded by a sheath of surfactant molecules which are adsorbed to the particle surface. They are included in the lubricant to prevent deposit formation on the metal engine parts and to neutralise acids. With the increased use of bio-diesel, an increase in the volume of small polar molecules (such as water and acetic acid) contaminating the lubricant has been observed. The mechanism of water interaction with overbased detergents has not been fully understood, however, it is known that water hinders their efficacy.

The effect of water on the overbased detergent is largely determined by the interactions between the water and the surfactant molecules. When water was added to samples of salicylate overbased detergents, sedimentation of surfactant and some metal carbonate occurred in the following 24 hours. Upon the addition of water to solutions of a particular overbased detergent in *n*-dodecane, gelling occurs over a period of weeks. The dynamics of gelling and mechanical properties of the gel have been found to vary depending on the volume fraction of particles and the volume of water added. This system has been studied by dynamic light scattering (see fig. 1), small angle neutron scattering. The gels have been characterised using controlled stress rheology and thermogravimetric analysis; results have shown different compositions and rheological properties at different sample heights. The arrest is hypothesised to be due to a depletion interaction, induced by the formation of aggregates of surfactant [1]. Varying the particle volume fraction, volume of contaminant and free surfactant concentration have all been found to have an impact on the arrest.

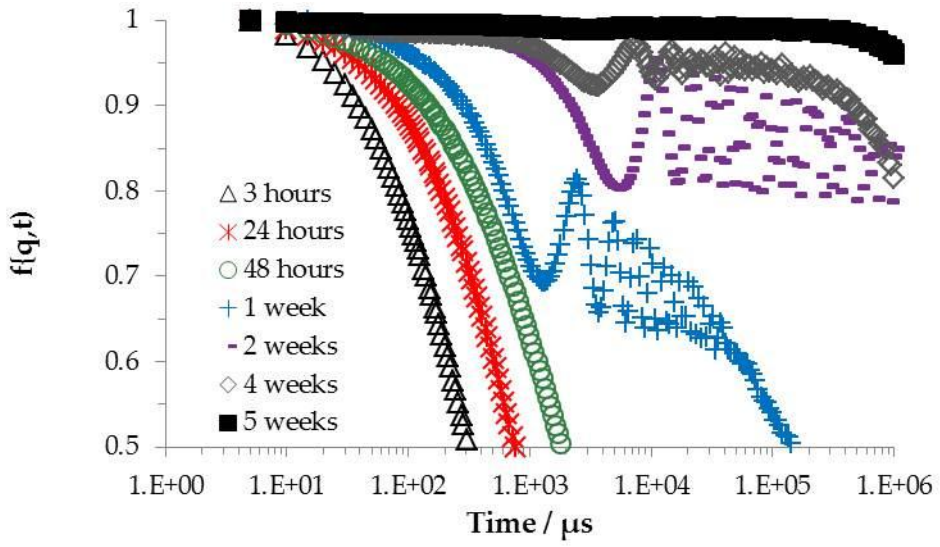

Fig. 1. Normalised intensity correlation functions, f(q,t) of one gelling sample over 5 weeks.

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Self-assembly, biomimetics and pattern formation

P.38 Lattice model of nucleation via partially disordered precursor

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[1]Centre for Complexity Science, University of Warwick, UK, [2]Department of Physics, University of Warwick, UK

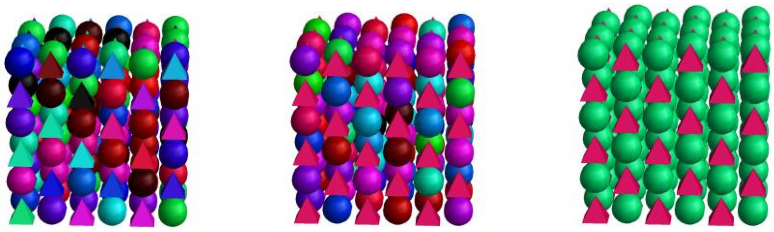
Nucleation is considered one of the fundamental mechanisms of phase transitions and has been studied for over a century in a broad range of systems. The study is largely motivated by the importance of control of not only the rates of phase transitions but also the size, morphology and other properties of the products of nucleation. Despite the large volume of experimental, theoretical and numerical findings, a number of key questions in nucleation theory, e.g. those regarding rates [1], pathways [2] and control strategies [3], remain open.

The process of biomineralisation, whereby nucleation and growth are mediated by organic components, appears to progress with a high degree of precision [4], which serves a natural example of self-assembly – a phenomenon of great technological interest [5]. The prototypical system for study of biomineralisation and polymorph selection is calcium carbonate ($CaCO_3$), where some degree of controlled assembly has been demonstrated in a laboratory [6–8]. Recently [9], it has been shown that crystallisation of calcite – the most stable polymorph of CaCO3 at ambient conditions – may proceed via an amorphous precursor followed by vaterite – a metastable polymorph whose molecular structure is characterised by a degree of structural disorder [10].

Some important insights into nucleation of $CaCO_3$ have been gained through molecular dynamics (MD) simulations [11–13], however, detailed atomistic models tend to be prohibitively expensive to probe the process directly. More rigorous studies [14–16], have used lattice models to show existence of amorphous precursors in assembly of anisotropic particles. To our knowledge, however, the amorphous and partially disordered precursor pathway has not been previously captured.

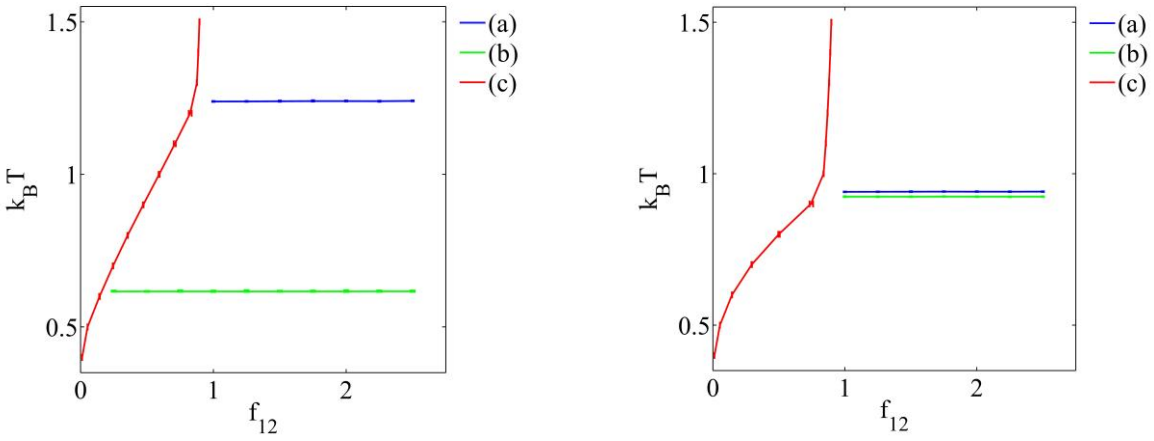
In the following contribution we present a lattice model of nucleation from solution, where the solute may take disordered, ordered or semi-ordered forms. We further show that, in the limit of slow growth, the transition from solvent rich to ordered crystalline state proceeds via the two polymorphs.

We study a three component system in semigrand ensemble on a cubic lattice with diagonal neighbour anisotropic interactions. We choose interactions which allow us to control the stability of the partially disordered polymorph and obtain corresponding phase diagrams using a variant of the Wang-Landau method [17] and histogram reweighting. By applying equilibrium path sampling [18], we show that the degree of disorder in solute nuclei, grown under moderate subcoolings and supersaturations, varies with their size.



(a) Disorder (D) (b) Partial disorder (PD) (c) Order (O)

FIG 1: Solute polymorphs



(a) Unequal anisotropic interactions

(b) Equal anisotropic interactions

FIG. 2: Phase diagrams for different anisotropic interaction strengths, where f_{12} is the solute saturation parameter. Coexistence lines shown: (a) D and PD; (b) PD and O; (c) solute and solvent.

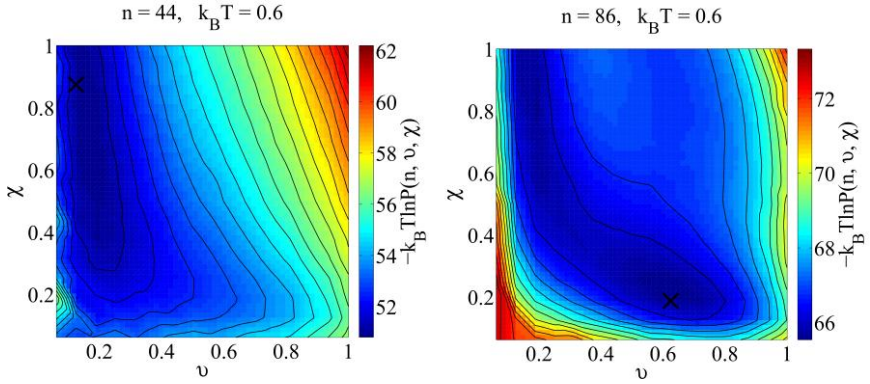


FIG. 3: Projections of free energy surfaces onto (v, x) plane, showing the transition of the local minimum from total disorder to partial disorder. Here n is the number of particles in the largest cluster present in the system, while v and x are parameters characterising the degree of orientational order within the cluster. The two orientational order parameters are such that state v = 1; x = 1 corresponds to perfect order, state $v \approx 0$; x = 1 - to disorder and state v = 1; $x \approx 0$ – to partial disorder. Contours are drawn at intervals of 1:0k_BT and black cross shows the coordinate of the local minimum.

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P.39 Fibrous scaffolds for neural tissue engineering in the auditory system

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At present, some types of hearing impairments have a palliative treatment whereas some, especially for those where otic neurons are damaged, cannot be properly treated. Recent findings had shown it possible to use human embryonic stem cell-derived otic neural progenitors (ONPs) as a new mode of treating hearing loss caused by damage to the spiral ganglion neurons (SGNs). To improve the efficiency and overcome some limitations of this treatment, the concept of tissue engineering, which involves an interaction between cells and scaffold, the matrix-mimicking construct, should be applied. Here, we describe the influence of poly(l-lactic acid)(PLLA) aligned fibers on ONP cell morphology, proliferation, neuronal differentiation and establishment of neural polarity in both progenitor and neuralising conditions. Furthermore, the PLLA fibers can be surface functionalized using amphiphilic block copolymers of poly(lactic acid)(PLA)-poly(2-methacryloyloxyethyl phosphorylcholine) (PMPC) and poly(lactic acid)(PLA) - poly[oligo (ethylene glycol) methyl ether methacrylate] (POEGMA) to generate cell inert hydrophilic fibers. By conjugating cell adhesive peptides such as RGD to the hydrophilic block (e.g. POEGMA), could be enhancing both cell adhesion and alignment.

P.40 Hierarchical morphogenesis of a hybrid peptide/protein system

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Tissue morphogenesis into hierarchical structures is a highly complex process from fast subcellular rearrangements to slow structural changes at the macroscale. Fundamental to this process are physical forces that are generated through dynamic physico-chemical interactions. The fabrication of functional macroscopic materials that can be morphed into complex shapes through directed and dynamic self-assembling mechanisms that mimic those found

in tissue development has not been achieved. Here we report the development of a dynamic peptide/protein self-assembling system that through emerging physico-chemical mechanisms is able to generate and dissipate stresses to undergo morphogenesis into complex hierarchical shapes with spatio-temporal control and in real time.

Our results demonstrate that the combination of a highly collapsed Elastin-Like Polypeptide (ELP) with a self-assembling amphiphilic peptide (PA) can spontaneously form dynamic macrotubular structures. This interfacial supramolecular system has the capacity to grow, controllably disassemble, adhere and seal to surfaces, be manipulated in real time, self-heal, and self-organize into complex macroscale geometries with nanoscale order. Morphogenesis into tubular structures was dependent on ELP and PA sequence, experimental setup, electrostatic and hydrophobic interactions, and temperature. In addition to undergoing morphogenesis, tubes exhibited elasticity and could be handled and manipulated.

Our system was used to generate robust and dynamic tubular networks by directed self-assembly without the use of predefined moulds. The interfacial phenomena reported here may provide a novel material fabrication platform for developing a new kind of hybrid peptide/protein nanomaterials with potential use in tissue engineering, biosensors, and electronic devices.

P.41 Synthetic DNA viruses for targeting breast cancer cells

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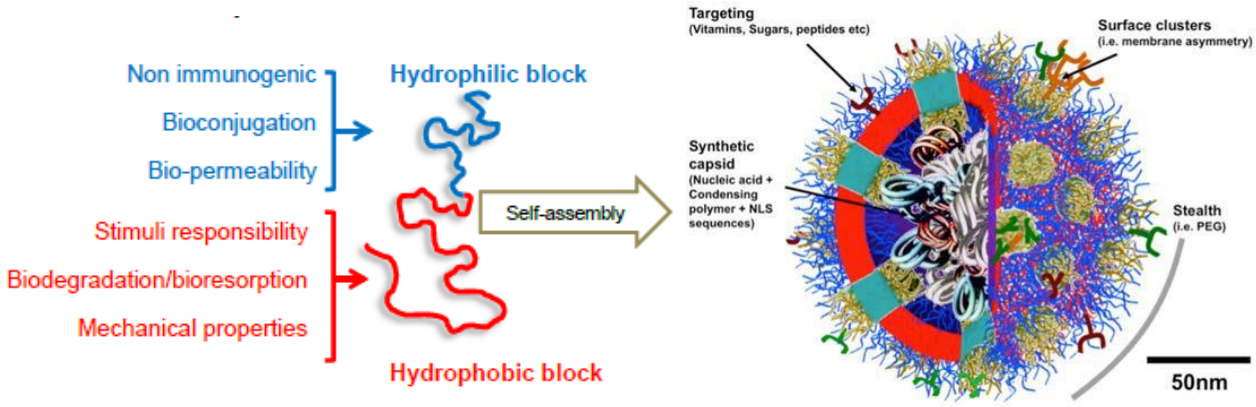
Breast cancer is the third most common cancer to cause deaths in all population and the second in women in UK, but with much lower 5 years survivals rates than other developed countries. Although enhanced permeability and retention (EPR) effect was previously demonstrated in anti-cancer macromolecules delivery in a tumor selective manner [1, 2], vectors that are highly selective and well permeable into tumors are strongly desired for early detection, diagnosis and clinical treatments. Since the statement of genetic central dogma [3] has made the gene function studies possible [4], such vectors are hoped to be potentially applicable in genetically affected diseases with efficient nucleic acids (NAs) delivery into targeted cells. As the most powerful tools in DNA transfection [5], viruses are excellent models to mimic for synthetic non-viral vectors design. Since late 90s, polymersomes have been proposed as platform for drug delivery systems [6, 7]. Polymersomes are closed vesicles (40-400nm in diameter) produced from the self-assembly of amphiphilic block copolymers in aqueous solution, which could be designed to be biocompatible and potentially biodegradable [8]. Considering their relatively robust membrane, kinetic stability, and stealth property, polymersomes were suggested to be more promising in the intercellular or intracellular delivery of macromolecules in live cells, and the determination of micro-studies compared to natural lipids [9].

Herein, we are aiming to discover the most optimal synthetic vectors to target breast cancer cells both *in vitro* and *in vivo,* and efficiently deliver DNA and/or DNA complex into nucleus as a new method to treat breast cancer by mimicking the natural viral infections. Breast cancer cell targeting will be achieved by conjugating specific ligands onto the polymersome surface at suitable intensity, while encapsulated DNA is decorated with condense components and nuclear localization sequence for nucleus entry.



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P.42 Design of patchy polymersomes with topological surface patterns at the nanoscale

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In Nature, biological membranes are composed of several components, which have been found to display nanometer and micrometer surface domains, called “rafts”.[1] Such domains play an important role in many biological processes such as cellular signaling, membrane trafficking and membrane modeling. To unravel the molecular basis and role of lipid surface domains in these processes, giant unilamellar vesicles have been widely studied as a mimicking system.[2]

Our research rather focuses on the design of complex artificial systems using synthetic membrane forming diblock copolymers as main constituents, because of their known enhanced mechanical properties and stability. These polymeric systems, a.k.a. polymersomes have recently yielded vesicles with patterned surfaces, using binary mixtures of diblock copolymers. Their surface topology could be controlled by the molar ratio of both block copolymer chains as well as their molecular weight. [3,4] However, it was observed that such systems evolve upon ageing towards asymmetric polymersomes, where phase segregation of diblock copolymers occurred.

To slow down this phenomenon, we propose to combine a diblock copolymer AB and a triblock copolymer ABC to prepare patchy polymersomes. In that case, the triblock copolymer would stabilize the patterns within the membrane, thus acting as a lineactant. To validate this concept, series of polymersomes made of PMPC-PDPA and PMPC-PDPA-PEO were prepared and characterized using TEM, DLS and cryo-TEM. Systematic analysis using FFT filtering was performed on the images to estimate the size of patterns and their evolution over time.

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P.43 Fabrication of "intelligent nanosurfaces" for controlled cell- substrate interaction

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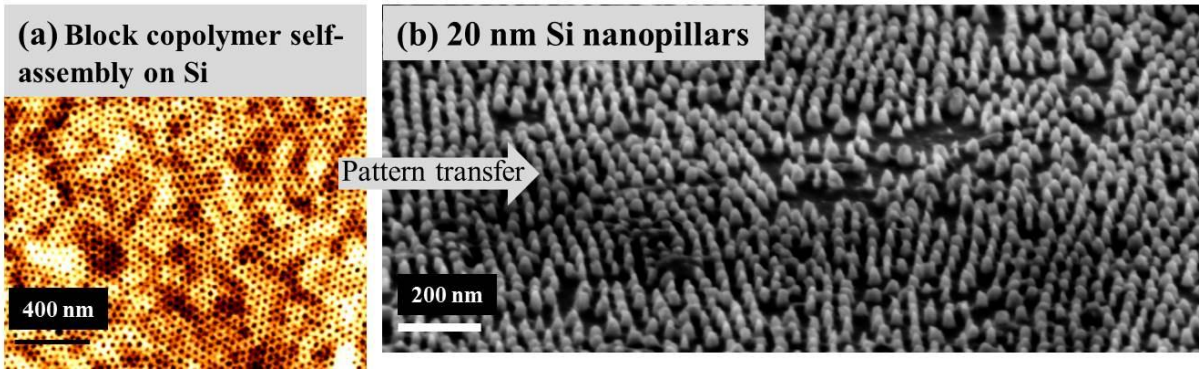
Neuroelectrodes are susceptible to deterioration via scar encapsulation following implantation. “intelligent nanosurfaces” which mimic the biological length scale may prevent this deterioration via the modulation of protein adsorption and cell adhesion. Furthermore nanotopography may significantly enhance electrode performance via enhanced charge transfer. A paradigme of nanobiomimetic design is that topographical features with dimensions similar to those of surface bound proteins (~10 nm) can significantly affect protein adsorption and cellular activity. However, the gold-standard for ordered nanofeature fabrication is E-beam lithography which is very expensive and time consuming. Furthermore, biological-dimension (sub-30 nm) feature size cannot be easily achieved. We describe a self-assembly process for the production of aligned and dense arrays of silicon nanopillars and nanowires using block copolymers. By modifying the shape and size of the nano features they act as functional materials for mimicking the natural biological architecture. We discuss the effect of the surface modifications on cell- substrate interaction in vitro and how they may enhance electrode charge transfer and improve neuron/electrode integration via modulation of the peri-electrode scar.



P.44 Artificial DNA membrane nanopores

K Göpfrich[1], T Zettl[1], J R Burns[2], V V Thacker[3], S Hernández-Ainsa[1], N A W Bell[1], E Stulz[3], S Howorka[2] and U F Keyser[1]

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Membrane nanopores are essential components of biological and artificial cells. Our group has shown that we can create artificial nanopores using DNA origami self-assembly [1], [2] and anchor them in lipid membranes [3]. Insertion of negatively charged DNA pores into a hydrophobic membrane is achieved by attaching functional hydrophobic groups in strategic positions on the DNA nanopores. Pore formation in lipid vesicles is studied for different nanopore designs and hydrophobic modifications via fluorescent imaging [4]. We demonstrate membrane anchoring using only two porphyrin-based lipid anchors. The porphyrin moieties also act as fluorescent dyes to aid the microscopic visualization of the DNA nanopore [3]. Single-channel current recordings of our artificial DNA nanopores are performed using a high-throughput lipid nanobilayer system that has recently been introduced by our group [5], [6]. Pore architecture and functionality of our DNA nanopores can be easily adapted, opening the pathway to design novel membrane channels.

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P.45 Out of equilibrium pattern formation in lipid membranes

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Artificial lipid bilayers are useful models of biological membranes, appealing for applicative purposes, and an interesting example of quasi-2D liquid systems on which to investigate new physics. It is well known that ternary-component lipid membranes, depending on the relevant thermodynamic parameters (composition, temperature and pressure), can show phase coexistence between two liquid phases, *Lo* and *Ld*, that can be imaged by fluorescence microscopy.

We have performed experiments observing both equilibrium and non-equilibrium morphology of lipid phases. Specifically we have investigated a new dynamical regime in which we follow the diffusive mixing of miscible phases, and observe pattern formation out of equilibrium. This has been possible thanks to the development of a method to induce rapid and spatially localized temperature changes, by infrared irradiation. In this fashion, a temperature change can be imposed faster (in about 1s) than the diffusive time over relevant lengthscales of a few microns (several 10s).

Our observations show that the line tension very rapidly vanishes upon heating the system above the miscibility transition temperature and after a few seconds the spectrum of the interface fluctuations becomes very different from the equilibrium capillary waves, growing in amplitude and losing the characteristic 1/wave-vector2 equilibrium form. The initial temperature change causes the less viscous phase to expand into the more viscous one promoting the roughening of the interface with a predominant lengthscale consistent with the wavelength of maximum instability in viscous fingering. The interface from then blurs out due to diffusion until the phases are fully mixed.

The same fast temperature change also allows us to very rapidly cool the system. This extends previous measurements by other groups, giving insight into processes that take place over the first few seconds of phase separation.

Investigating the aspect of pattern formation on lipid bilayers is relevant because lipid membranes, for their remarkable physical properties, are considered an interesting building block for the design of novel soft materials. The possibility of being able to construct blocks with user-defined pattern and the ability to control pattern formation would be highly desirable for tuning their self-assembly properties.

Surfactants, foams and emulsions

P.46 Surfactants and aqueous solubility enhancement of drugs: importance of the hydrophilic "head group"

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Micellar solubilisation is an attractive way of increasing the apparent aqueous solubility of poorly-water soluble drugs. While the effect of increasing the alkyl chain length of a surfactant (SAA) on solubilisation is well understood, very little is known about the effect of changing the nature of the hydrophilic head group. Accordingly, we report here on systematic studies performed to determine the solubilisation capacity of micelles formed by a range of C_{12} chain surfactants (SAAs) with varying head groups, namely the cationic dimethylammonium bromide (TAB), the anionic sodium sulphate (SS), the zwitterionic dimethylamminopropanesulphonate (DAPS), the phosphocholine (PC), the dimethylamine-N-oxide (DAO) for the poorly-water soluble drug, testosterone propionate (TP).

The solubilisation capacity of the various micelles for TP was correlated with the structure of the micelles. Micelle structure, in the absence and presence of saturation amounts of TP, was determined using small angle neutron scattering (SANS) in combination with contrast variation. For the micellar systems tested, three 'contrasts' namely, protiated SAA (h-SAA) in D_2O, chain-deuterated SAA (d-SAA) in H_2O and d-SAA in D_2O were studied. The critical micelle concentration (CMC) of the SAAs was determined by surface tensiometry. As the CMC of the SAAs are very low in comparison to the concentrations used for the solubilisation and SANS studies, their contribution to the measurements were assumed to be negligible. Furthermore, as the aqueous solubility of TP is only 0.0009 %w/w, any increase in the apparent solubility of TP in the presence of micelles assumes that the TP is present in the surfactant micelles.

The studies show that the SAA head group plays a significant role both on the structure of the micelles and their capacity to solubilise TP. For example, the SANS studies showed that, at saturation, the charged surfactants, particularly C_{12}SS, exhibited the greatest capacity for TP, and the non-ionic micelles the least, with the micelle formed by the zwitterionic surfactants being intermediate. Furthermore, regardless of head group, all micelles were prolate in shape and became even more elongated in shape in the presence of TP. This study suggests that surfactant charge is important in solubilising TP, even though TP is neutral. Further studies (MD simulations and neutron reflectivity) are underway to determine the precise location and/or orientation of TP within the micellar systems above.

P.47 Pickering emulsion by arresting phase separation using anisotropic particles

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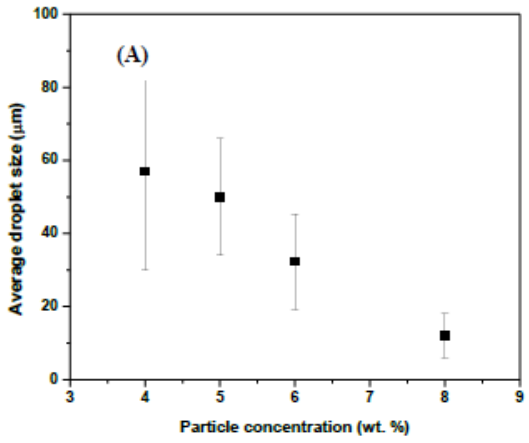
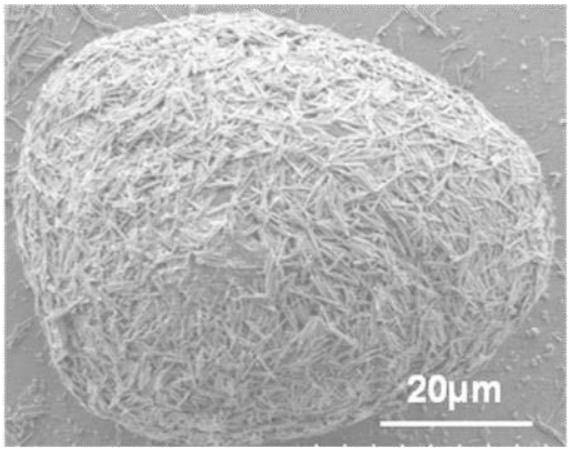
The phase separation induced by heating or cooling of a binary fluid mixtures having an upper or a lower critical solution temperature respectively, can be arrested by incorporating colloidal particles before initiating phase separation. The ability of colloidal particles to arrest phase separation in such systems has been recently exploited to create emulsions of complex morphologies – namely Bijels [1-3]. In current work, we exploit the colloidal interactions of interfacially trapped shape anisotropy particles to arrest phase separation in a phase separating binary liquid mixture. We show that colloidal rod-stabilized Pickering emulsions can be by obtained by arresting phase separation in lutidine-water (L-W) binary liquid mixture. In a typical experiment, a single phase homogenerous L-W mixture (at critical composition) containing silica rods was prepared. This solution was heated to a temperature above LCST (43°C) at a controlled heating rate of 28°C/min to induce phase separation. During the phase separation process, the particles migrate to the additional interface area created and hence stabilize the interface. As a consequence spherical droplets of emulsion were formed. Emulsion droplet size can be tuned by varying the particle concentration. The decrease in droplet size with increasing particle concentration follows the predictions of the limited coalescence phenomena.



A)



B)

Fig. 1 (A) Effect of particle concentration on average droplet size - Average emulsion droplet size and droplet size polydispersity decreases with increasing particle concentration. Fig. 1 (B) Scanning electron micrograph of dried non-spherical water droplets stabilized by colloidal rods - obtained when a dispersion containing 4 weight % of rod shaped silica particle (AR ~ 5) in L/W mixture was heated from the temperature of 30° C to 43 °C at a maximum heated rate of 13 °C/min.

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P.48 Immiscible lipids control the morphology of patchy emulsions

L-L Pontani

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We study the phase behavior of immiscible mixtures of phospholipids and cholesterol at the interface of oil-in-water emulsions. Such mixtures spontaneously decompose into domains on the surface of droplets, similar to the formation of lipid rafts in cells. Using a microfluidic device we control the production of monodisperse emulsions and map out a ternary immiscibility diagram allowing for the control of various surface morphologies, including spots, stripes, and hemispheres. While bilayer membranes require ternary mixtures for domain formation, all morphologies are found to be accessible using only binary mixtures of either cholesterol and DOPC or cholesterol and sphingomyelin on emulsion monolayers. By functionalizing those controlled patterns with biotinylated lipids, we also make useful candidates for directed self-assembly with specific interactions via streptavidin.

Using confocal microscopy and image analysis we find that domains grow to a maximum size and then remain stable against coarsening on a timescale of weeks. Surprisingly stability is not compromised by the presence of increasing amounts of salt, indicating that the stabilizing force is not electrostatic in origin. We investigate and discuss the potential driving forces for the stability of the domains and note that different lipid compositions could lead to different stabilization mechanisms.

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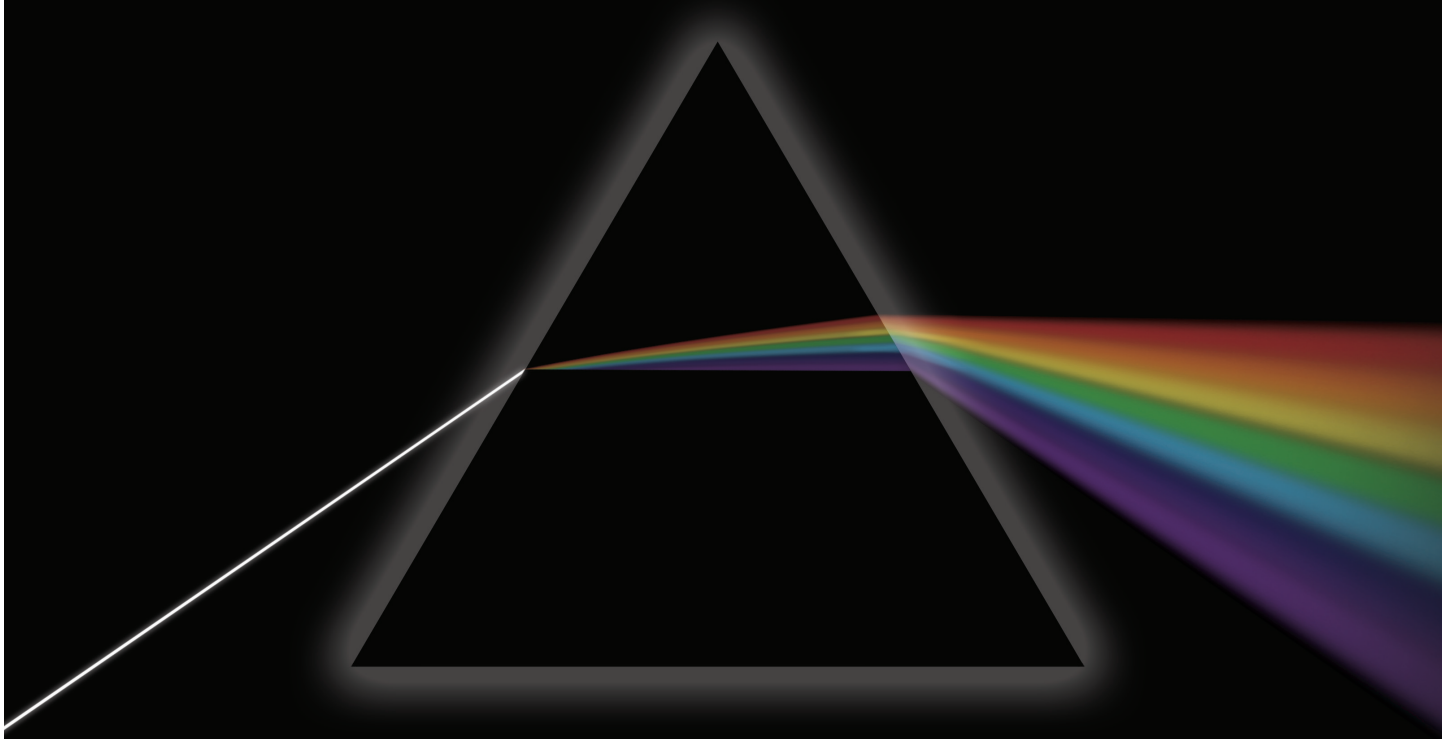

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