

Abstract Book



2nd WORKSHOP on Complex Liquids at Structured Surfaces theory meets experiment

Lisbon, 10-12 October 2012

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Jointly organized by:

Centro de Física Teórica e Computacional da Universidade de Lisboa, Portugal

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2nd WORKSHOP ON COMPLEX LIQUIDS AT STRUCTURED SURFACES

Programme - Wednesday, October 10

Superhydrophobicity

8:45 - 9:00 Opening remarks

Chairperson: P. Teixeira

9:00 - 10:00 **C. Cottin-Bizonne (Invited)**
Slippage of simple liquids past super-hydrophobic surfaces

10:00 - 10:30 **M. Popescu (Invited)**
Buoyancy driven small drops or air bubbles colliding with fluid-fluid interfaces

10:30 - 11:00 Coffee Break

Chairperson: B. Ocko

11:00 - 12:00 **M. Brinkmann (Invited)**
Wetting of regularly structured substrates

12:00 - 12:30 **A. Checco**
Liquid infiltration and air trapping into hydrophobic nanocavities

12:30 - 14:00 Lunch Break

14:00 - 16:00 **Discussion led by A. Checco**
Superhydrophobic surfaces and flows over heterogeneous solids

16:00 - 16:30 Coffee Break

Self-assembly

Chairperson: M. Tasinkevych

16:30 - 17:30 **F. Martinez-Veracoechea (Invited)**
Targeting and self-assembly using super-selective nanoparticles

17:30 - 18:00 **A. Tkachenko**
Programmable self-assembly of DNA-nanoparticle mesostructures

18:00 - 18:30 **B. Ocko**
Surface induced order in molecular and polymer systems

2nd WORKSHOP ON COMPLEX LIQUIDS AT STRUCTURED SURFACES

Programme - Thursday, October 11

Self-assembly

Chairperson: J.M. Tavares

- 9:00 - 10:00 **P. Poulin (Invited)**
Self-assembly of carbon nanotubes for thin conductive films
- 10:00 - 10:30 **O. Gang**
Nanoscale self-assembly guided by DNA and geometry: Structures, transformations and rational design
- 10:30 - 11:00 Coffee Break

Chairperson: M. Rauscher

- 11:00 - 11:30 **A. Law**
Self-assembly of two-dimensional colloidal clusters
- 11:30 - 12:00 **A. Maciolek**
Phase behaviour, structure and aggregation of colloids immersed in near-critical solvents
- 12:00 - 12:30 **N. Bernardino**
Re-entrant wetting of network fluids
- 12:30 - 14:00 Lunch Break

Chairperson: N.G. Almarza

- 14:00 - 15:00 **F. Sciortino (Invited)**
Colloidal self-assembly of triblock Janus particles and other patchy colloids
- 15:00 - 15:30 **D. de Las Heras (Invited)**
Bicontinuous and mixed gels in binary mixtures of patchy colloids
- 15:30 - 16:00 Coffee Break

Chairperson: Y. Kalyuzhnyi

- 16:00 - 16:30 **M.M. Telo da Gama (Invited)**
Self-assembly of anisotropic particles: nematic and patchy colloids
- 16:30 - 18:30 **Discussion led by M.M. Telo da Gama**
Colloidal self-assembly and interactions with surfaces
- 20:00 - 22:00 Workshop dinner

2nd WORKSHOP ON COMPLEX LIQUIDS AT STRUCTURED SURFACES

Programme - Friday, October 12

Liquid crystals at patterned surfaces

Chairperson: N.M. Silvestre

- 9:00 - 10:00 **D. Aarts (Invited)**
Confined colloids: rods and spheres
- 10:00 - 10:30 **A. Parry (Invited)**
Capillary condensation revisited: two Kelvin equations
- 10:30 - 11:00 Coffee Break

Chairperson: P. Patrício

- 11:00 - 11:30 **J.M. Romero-Enrique (Invited)**
Theoretical characterization of the surface free energy of a nematic in contact with microstructured substrates
- 11:30 - 12:00 **V. Reshetnyak (Invited)**
Frederiks transition in ferroic liquid crystal suspension
- 12:00 - 12:30 **M. Blow**
Switching between nematic filled states: flexoelectric and order-electric coupling
- 12:30 - 14:00 Lunch Break

Chairperson: V. Choliy

- 14:00 - 15:00 **J. Yeomans (Invited)**
Stirring by microswimmers
- 15:00 - 15:30 **M. Tröndle**
Chemically patterned surfaces and critical Casimir forces
- 15:30 - 16:00 Coffee Break
- 16:00 - 18:00 **Discussion led by S. Dietrich**
Patterned surfaces and complex fluids
- 18:00 - 18:30 Concluding remarks

TALKS & DISCUSSIONS

Slippage of simple liquids past super-hydrophobic surfaces

C. Cottin-Bizonne

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Reducing the friction of liquid flows at solid boundaries has become an important issue in the context of the development of microfluidic systems. The use of gas as a lubricant – such as microbubbles trapped in super-hydrophobic surfaces – is commonly suggested as a possible way to achieve high slippage of liquids at walls. This presentation will focus on the characterization of slippage of simple-liquid flows over super-hydrophobic surfaces with a short review on theoretical and experimental studies (including μ -PIV - Particule Image Velocimetry - and nanorheology measurements). Scaling laws quantifying the super-lubricating potential of super-hydrophobic nano/micro patterned surfaces will be presented and compared with numerical and experimental studies. The influence of the pattern geometry (such as periodicity, fractal surfaces) and of the curvature of the liquid-gas menisci on the hydrodynamic boundary condition will be emphasized regarding the actual capacity of liquid-gas interfaces at super-hydrophobic surfaces to reduce slippage.

Buoyancy driven small drops or air bubbles colliding with fluid-fluid interfaces

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By combining microfluidic methods for producing drops or bubbles with sizes in the few hundred micron range with high-speed video microscopy, we have been able to perform systematic studies of the buoyancy driven motion at low Reynolds numbers of small drops or air bubbles through simple or complex liquids, as well as their collision with quasi-planar fluid-fluid interfaces. Here we focus on the latter process, i.e., the approach to, and collision with, the interface.

As a particular example, we will discuss a potentially new method for determining tight lower and upper bounds for the electrical potential of certain fluid-fluid interfaces. The value of the electric potential (or that of the closely related "zeta"-potential [1]) of a liquid-fluid (i.e., liquid or gas) interface is a crucial parameter for, e.g., the stability of emulsions which are extensively used in the food, cosmetics, or pharmaceutical industries [2]. Because such interfaces are deformable, determining their zeta-potential remains a challenging task [2].

We exploit the spontaneously occurring cascade partial coalescence [3] of a drop of heptol (toluene - n-heptane mixture) rising through water (electrolyte) with a water (electrolyte) - heptol quasi-planar interface, process in which a stable drop emerges as the final state, to estimate lower- and upper-bounds (calculated within the classic DLVO theory [1]) for the absolute value of the electric potential of the oil - water (electrolyte) interface.

References

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Wetting of regularly structured substrates

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Despite the enormous amount of literature published on superhydrophobicity, the wetting of non-flat, moderately hydrophilic surfaces is still barely addressed [1]. A theoretical approach to establish a link between contact angle hysteresis or droplet eccentricity on anisotropic patterns, and the geometry of the surface features is still missing. In order to elucidate the fundamental relation between advancing contact angles and substrate geometry, a highly idealized system consisting of a plane surface decorated with a regular array of posts with circular cross section is investigated using numerical minimizations of the interfacial energy. Employing the static apparent angle as a control parameter, a number of interfacial instabilities are detected, which lead to topological transitions of the interface and contact line. Such instabilities can be depinning from sharp edges, coalescence of the liquid menisci ahead of the posts, or the appearance of soft deformation modes of the interface. By extensively varying the line fraction and aspect ratio of the posts as well as the material contact angle of the substrate, a complete numerical characterization of the system is constructed [1]. The second part of the talk will be devoted to a study of global equilibrium shapes of droplets in contact to a regular pattern of linear grooves with triangular cross section. Depending on the opening angle of the grooves and the material contact angle, the liquid either spreads only into the directions of the grooves, or grows into all three dimensions. In the latter case, the droplet approaches a scale invariant shape as the number of covered grooves increases. A mapping of the shape to a partially wetting droplet on a plane linear stripe can be employed to predict the droplet eccentricity in this asymptotic limit. As this model is not restricted to a specific class of patterns, it can be applied through suitable mapping to any type of chemical or topographic pattern. On all of these linear surface patterns, shrinking droplets exhibit an almost circular shape.

References

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Liquid infiltration and air trapping into hydrophobic nanocavities

Antonio Checco

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The infiltration of water and various organic liquids into hydrophobic nanocavities (~20 nm wide and 100-160 nm deep) is studied using transmission small angle x-ray scattering. The results indicate that the infiltration depends on the liquid surface tension and wetting contact angle. Furthermore, a significant amount of air remains trapped into the cavities, regardless of the liquid's wetting angle. The volume of the resulting nanobubbles is compared to a simple model where the liquid capillary pressure is balanced by the bubble internal pressure. The importance of microscopic effects such as contact line pinning and disjoining pressure is also discussed.

Superhydrophobic surfaces and flows over heterogeneous solids

Discussion leader: A. Checco, Brookhaven National Laboratory, U.S.A.

The discussion will address, but not be limited to, the following:

- Equilibrium Wenzel and Cassie states and the thermodynamic transitions between them as determined by the size and type of substrate texture, i.e., the distribution of features and the feature size.
- Dynamic Wenzel to Cassie transition, including contact line pinning, as determined the substrate texture.
- Dynamics of the precursor film and its dependence on the substrate geometry and chemistry.
- Liquid flow over uniformly textured substrates with inhomogeneous chemical composition (gradients): transverse velocity components or anisotropic effective slip?

Targeting and self-assembly using super-selective nanoparticles

F. Martinez-Veracoechea

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A long-standing goal of Soft Matter Physics is to understand how constructs of arbitrary complexity can be formed through self-assembly of nano-building-blocks. In principle, such constructs could act as smart and functional nanodevices with potential applications across a variety of disciplines including Biology, Medicine, Nanotechnology, and Engineering. An important step towards building complex nanodevices has been made with algorithmic [1], generation-by-generation assembly. In this scheme, the components of the target structure are made to self-assemble in an orderly fashion by carefully providing kinetically favourable pathways to the thermodynamically stable state.

In order to generalize such assembly strategies, one must first obtain excellent control over the binding events between the different docking sites on the nano-building blocks. More precisely, we need to design nanoparticles that can target a given surface or nano-object, and do so selectively in the presence of other surfaces with competing binding interactions. Besides being useful for self-assembly, such “super-selective” targeting has immediate implications for nano-medicine, as one could fabricate devices that can treat individual target cells (e.g., cancer cells) without affecting the healthy ones. Indeed, nano-targeted delivery is an active area of research [2], as it has been found that cancer cells tend to overexpress certain membrane receptors in comparison with healthy cells. [3] However, to exploit this distinction between target and healthy cells, one must design nanoparticles that only bind to surfaces displaying an above-threshold coverage of a particular receptor, while leaving other surfaces intact.

Using computer simulations and a simple analytical model, we have shown that this kind of super-selectivity can be obtained with multivalent nanoparticles, which use a large number of intervening ligands that simultaneously bind to surface receptors [4]. The main idea is that in multivalent particles the number of binding arrangements rapidly increases with the number of receptors on the target surface, causing a sharp dependence of the particle’s binding free energy with receptor concentration. In effect, such particles exhibit a nearly “on-off” behaviour ideal for specific targeting. However, while this simple model accounts for the complex interplay between valence, binding strength and bulk concentration observed in systems of multivalent nanoparticles, a number of questions must still be addressed before such particles can be reliably used in real nano-technology applications. Finally, we present simulation results that shed light on the way to address some of these questions.

References

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Programmable self-assembly of DNA-nanoparticle mesostructures

Alexei V. Tkachenko

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In recent years, an impressive progress has been made in using the molecular recognition properties of DNA to control self-assembly of nanoparticles (NPs) into variety of DNA-NP supercrystals. Self-assembly of finite size DNA-NP structures have received much less attention. Such programmable NP clusters would open new opportunities in a variety of fields where bottom-up assembly of 3D nano-objects with well defined composition and architecture is required, e.g. nanoplasmonics, nanomedicine, metamaterials. In my talk, I will show that a variety of target mesoscopic structures, each with a programmed local morphology and complex overall shape, can be self-assembled at a near perfect yield. The proposed building blocks, octopus NPs, are inspired by recent proof-of-principle experiments in which DNA were attached at specific locations on the particles. We introduce the methodology for solving the inverse problem in self-assembly, i.e. designing building blocks that assemble into an arbitrary desired structure, in a robust manner. The design method is then verified by simulating the self-assembly of cubes, pyramids and even an Empire State Building model from an initially homogeneous solution of NPs. Our study demonstrates that one can completely avoid unwanted metastable configurations, and therefore the self-assembly occurs on relatively fast timescales determined primarily by particle diffusion and binding, but not by exploration of potentially vast configurationally space (as e.g. in protein folding problem).

Surface induced order in molecular and polymer systems

Ben Ocko

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We have carried out surface x-ray scattering measurements to determine the phase behavior of molecular and polymer systems in contact with solid walls and at the vapor interface. For molecular systems the interfacial interactions may give rise to surface freezing, where a single or double frozen layer is in contact with the bulk over a range of temperature. Our recent results at oxide surfaces show that the surface frozen temperature depends on the specific interactions with the interface. For ionic liquids, the surface induced ordering can extend from a single layer to many layers. In the case of conjugated polymers, nanoimprinting induces alignment and orientational order not found in the bulk. Recent results from the BNL Soft Matter Group and its collaborators will be presented.

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Self-assembly of carbon nanotubes for thin conductive films

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Carbon nanotubes (CNTs) are promising materials to develop novel conductive inks potentially useful in organic electronics for flexible circuitry or transparent electrodes. Indeed, carbon nanotubes exhibit a high aspect ratio, an excellent chemical stability and a high electrical conductivity. Because of their large aspect ratio they can form conductive networks at low concentration. The optical and electrical properties of thin films depend on the intrinsic properties of CNTs but also on their structuration on a given substrate. This structuration is imposed by the processing used to deposit CNTs from a fluid phase and on the interactions between the nanotubes.

We will discuss in this presentation some aspects related to the self-assembly of CNTs for the development of thin conductive films. A key objective for transparent electrodes is the control of the network morphology to combine high conductivity and optical transmittance. We will discuss in particular the influence of interactions between the CNTs. The latter affect the rheological, wetting and self-assembly properties of CNT dispersions. It is theoretically expected that weak attractive forces should promote local alignment of the CNTs along with a decrease of the percolation threshold [1, 2]. Local alignment should lead to better electrical contacts. We have recently validated these theoretical expectations. Cryo-TEM analyses show that increasing the surfactant concentration in the dispersion actually promotes contacts and local alignment of CNTs. Weak attractive interactions result in an increase of the ink viscosity which yields improvements of processability. For other applications, such as flexible circuitry, aligned and packed CNTs are preferable. CNT because of their aspect ratio can form liquid crystals which are well suited to form self-assembled anisotropic conductors. We will present recent results on the relationship between the order parameter of CNT liquid crystals and the electrical properties of CNT thin films [3].

References

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Nanoscale self-assembly guided by DNA and geometry: Structures, transformations and rational design

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The structural plasticity and tunable interactions provided by DNA chains offer a broad range of possibilities to direct the organization of nanoscale objects into well defined systems, as well as to induce the structural transformations on demand. We have studied the assembly of clusters and extended 2D and 3D array architectures from nanoscale components of multiple types driven by DNA recognition, chain effects and geometrical factors. Our work explores how DNA-encoded interactions between inorganic nano-components can guide the formation of well-defined superlattices, how the morphology of self-organized structures can be regulated in-situ, and what factors govern a phase behavior. The role of flexible chains, particle anisotropy, and external stimuli on a structure formation and its transformation will be discussed in details. I will also demonstrate the use of the discussed approaches for rational nanomaterial engineering.

Acknowledgement: *This research is supported by the U.S. DOE Office of Science and Office of Basic Energy Sciences under contract No. DE-AC-02-98CH10886.*

Self-assembly of two-dimensional colloidal clusters

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We study the structure of binary monolayers of large (3 μm diameter) very hydrophobic (A) and large (3 μm diameter) hydrophilic (B) or small (1 μm diameter) hydrophilic (C) silica particles at an octane/water interface. By tuning the composition and packing geometry of the mixed monolayer, we find that a rich variety of two-dimensional hexagonal super-lattices of mixed A/B or A/C clusters are formed, stabilized by short-ranged electrostatic induced dipole interactions. The cluster structures obtained are in excellent agreement with zero temperature calculations, indicating that the self-assembly process can be effectively controlled.

Phase behaviour, structure and aggregation of colloids immersed in near-critical solvents

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We study stability and thermodynamic properties of a colloidal suspension with a phase-separating solvent, such as a binary-liquid mixture with a miscibility gap. We focus on the near-critical region of a solvent, where the critical fluctuations drive the divergence of the correlation length. As a consequence, the adsorption properties of the colloids become important and the effective so-called critical Casimir forces (CCFs) acting between the colloids emerge. The range and the strength of the CCFs are easily and reversibly tunable by temperature and the bulk ordering field. Within an approach in terms of effective one-component colloidal systems we analyze colloidal aggregation due to CCFs and thus allude to previous experimental studies which are still under debate. Concerning the phase diagram, the phase segregation into two phases, one being rich and the other poor in colloidal particles, is investigated and the limitations of the effective approach, which is commonly used, are discussed.

Re-entrant wetting of network fluids

N. R. Bernardino and M.M. Telo da Gama

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We use a simple mesoscopic Landau-Safran theory of network fluids to show that a re-entrant phase diagram, in the “empty liquid” regime, leads to non-monotonous surface tension and re-entrant wetting, as previously reported for binary mixtures. One of the wetting transitions is of the usual kind, but the low temperature transition may allow the display of the full range of fluctuation regimes predicted by renormalization group theory.

Colloidal self-assembly of triblock Janus particles and other patchy colloids

F. Sciortino

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Colloidal particles have the right size to form ordered structures with periodicities comparable to the wavelength of visible light. Driven by the demands of several emergent technologies, efforts have been made to develop efficient, self-assembly-based methodologies for generating colloidal single crystals with well defined morphologies. Somewhat unfortunately, these efforts are often frustrated by the formation of structures lacking long range order; hard-sphere colloids, for example, crystallize into coexisting regions of face-centered cubic and hexagonal closed-packed structures. Inspired by recent developments in the synthesis and understanding of patchy colloids, we show that the rational design of patch shape and symmetry can drive the system to crystallize in a single, selected morphology by structurally eliminating undesired polymorphs.

References

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Bicontinuous and mixed gels in binary mixtures of patchy colloids

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We investigate the thermodynamics and percolation regimes of model binary mixtures of patchy colloidal particles. The particles of each species have three sites of two types, one of which promotes bonding of particles of the same species while the other promotes bonding of different species. We find up to four percolated structures at low temperatures and densities: two gels where only one species percolates, a mixed gel where particles of both species percolate but neither species percolates separately, and a bicontinuous gel where particles of both species percolate separately forming two interconnected networks. The competition between the entropy and the energy of bonding drives the stability of the different percolating structures.

Self-assembly of anisotropic particles: nematic and patchy colloids

M.M. Telo da Gama

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I review recent work at CFTC on (i) the interactions of nematic colloids and (ii) primitive models of patchy colloids in the bulk and close to surfaces. The relation between the two will be emphasized.

Colloidal self-assembly and interactions with interfaces

Discussion leader: M.M. Telo da Gama, CFTC Lisboa, Portugal

The discussion will address, but not be limited to, the following:

- Assembly of surface-textured colloidal particles ranging from patchy colloids to spherical colloids in ordered fluids, where the patches are equilibrium defects with very precise symmetries.
- Experimentally-validated models for the effective interactions and self-assembly of patchy colloids at fluid-fluid and solid-fluid interfaces.
- Dynamic behaviour of colloidal particles at, and in approaching/ passing through fluid-fluid interfaces.

Confined colloids: rods and spheres

D. Aarts

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The ongoing miniaturization in science and technology increases the importance of surfaces and boundaries and raises new questions about the behaviour of liquids in confinement. One particularly suitable way to study these emerging questions is by combining colloid science with soft-lithography techniques. We will focus on two problems. Firstly, we study the nematic phase of rodlike fd virus particles confined to channels with wedge structured walls. Here, we observe a splay to bend transition at the single particle level as a function of the wedge opening angle. Lattice Boltzmann simulations reveal the underlying origin of the transition and its dependence on nematic elasticity and wedge geometry. Our combined work provides a simple method to estimate the splay-to-bend elasticity ratios of the virus and offers a way to control the position of defects through the confining boundary conditions. Secondly, we study the fluid-fluid demixing kinetics and morphology of a system of spherical colloids and non-adsorbing polymers confined between two parallel walls. We follow the dynamics at the single domain level, which allows us to test the stability of the formed liquid bridges. Finally, we consider the role of hydrodynamics and of thermal interface fluctuations in our system.

Capillary condensation revisited: two Kelvin equations

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It is well known that a vapour, confined between two identical infinite parallel walls (with contact angle $\theta < \pi/2$), condenses to liquid, at a pressure below that of bulk saturation. This shift in the location of the first-order phase boundary, referred to as capillary condensation, is described by the macroscopic Kelvin equation, and has been extensively tested using microscopic DFT and simulation methods. In this talk we show that when one caps the capillary (so that the geometry is that of a long groove), the order of capillary condensation may be dramatically altered and is determined by the wetting properties of the capped end. If this is partially wet, capillary condensation remains first order while if it is completely wet, the condensation is continuous. The change in order of the condensation brings together several key ideas in the theory of wetting and corner filling transitions and is neatly summarised by a companion equation to the Kelvin equation, which determines the size of the metastable region.

Theoretical characterization of the surface free energy of a nematic in contact with microstructured substrates

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Nematic liquid crystal in presence of microstructured grooved substrates may show frustration in the orientational order, leading to elastic deformations in the nematic director field and in some cases the nucleation of topological defects. As a consequence, there is a contribution to the excess surface free energy associated to these elastic deformations. In the 70s, Berreman introduced a way to estimate this contribution for shallow substrates and when the nematic texture does not present topological defects. This approximation is qualitatively correct for nematics in contact with smooth substrates and no topological defects in the texture, but it fails in presence of cusped substrates, such as the sawtoothed and the crenellated gratings. We introduce a generalization of the Berreman expression when the nematic texture shows disclination lines, and we will discuss the effect of this contribution in wetting transitions.

Frederiks transition in ferroic liquid crystal suspension

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Liquid crystal colloids display a richer set of properties than conventional colloidal systems [1]. Of these, ferroelectric and ferromagnetic liquid crystal colloids have been the subject of considerable recent work [2-9]. The colloidal particles are so small that the suspensions seem optically identical to pure liquid crystal, but nevertheless the electric and magnetic field response is strongly enhanced, even at low colloidal concentrations.

Using continuum and statistical mechanical theories, we study the switching properties in a nematic liquid crystal cell doped with ferromagnetic particles subject to homeotropic boundary conditions at the cell and particle walls [8]. An external magnetic field normal to the cell plane is also imposed. At low fields we find thresholdless switching of the nematic director, consistent with experimental data. At higher fields, there are three regimes, depending on the strength of the anchoring interaction between the director and the ferroparticle orientation. For low anchoring strengths, there is an inverse Frederiks effect, and the nematic reorientation reduces and then disappears continuously at a critical magnetic field. At intermediate fields, the degree of reorientation reduces at high fields but remains finite. For high fields, however, the director switching saturates.

We also construct a theoretical model of the dielectric properties of a ferroelectric LC nanosuspension, using a generalized Maxwell-Garnett picture. The theory supposes that the suspension may as a first approximation be considered as a complex homogeneous dielectric ceramic, thus neglecting positional correlations of the colloidal particles. The suspension then consists of an anisotropic matrix with a very low concentration (<1% by volume) of impurity particles. The impurity particles possess both shape and dielectric anisotropy, as well as a permanent electric polarization and strong liquid-crystal director anchoring on the particle surface. We calculate the effect of doping a liquid crystal with ferroelectric impurities on the Frederiks transition. The theory takes account of inclusion shape, dielectric susceptibility, and local field effects. We neglect the possibility of dielectric particle chaining, which appears experimentally not to occur in general. Our calculations [9] suggest, in qualitative agreement with experiment, that doping a nematic liquid crystal with ferroelectric particles, even at very low particle concentration, can in some cases significantly shift the electric Frederiks threshold field.

Acknowledgement: *This work was partly supported by EOARD Grant 078001.*

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Switching between nematic filled states: flexoelectric and order-electric couplings

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Using numerical simulations, we model a nematic liquid crystal, in coexistence with its isotropic phase, filling a substrate patterned with rectangular grooves. We analyse its response to an externally-applied electric field, under flexoelectric and order-electric coupling, with an emphasis on identifying switching transitions between bistable morphological states. We identify that order-electricity provides a means of switching between states where the plateaux between grooves are dry and where they are wet by a nematic layer, without affecting the configuration of the nematic within the groove. We identify that flexoelectricity is a viable means of changing the topological configuration of the nematic in the groove, provided that the coupling differentiates between the type of distortion at the corners of the substrate. We determine precisely the field magnitudes and orientations required to effect each type of transition.

Stirring by microswimmers

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Because of their size bacteria and fabricated micro-swimmers swim at low Reynolds number, a regime where the effect of hydrodynamics can be counterintuitive. Moreover micro swimmers provide experimentally accessible examples of active systems that create their own energy and operate out of thermodynamic equilibrium.

The mechanisms by which bacteria interact with particles in their environment are relevant to their feeding strategies and may contribute to oceanic mixing. We discuss how passive tracers are advected by swimmers, and hence estimate the diffusion constant of particles in a bacterial suspension.

We also examine encounters between a swimming bacterium and an inert spherical particle across a range of particle sizes, from tracers, through particles of intermediate size that are capable of deflecting the paths of the bacteria, to particles much larger than the swimmer that effectively behave as curved surfaces as a swimmer approaches.

Chemically patterned surfaces and critical Casimir forces

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Colloids and substrates confining a (near-) critical fluid are subject to effective, solvent-mediated critical Casimir forces. The strength and the direction of these forces depend on temperature and the chemical properties of the surfaces. Thus, patterning surfaces with stripes of different chemical properties leads to a rich behavior of the critical Casimir effect.

▲ Colloids near chemically patterned substrates are subject to laterally confining potentials and may form highly ordered colloidal assemblies [1].

▲ A suitable choice of chemical stripes forming the pattern may lead to levitation of colloids at a stable distance from the substrate induced by critical Casimir forces [2].

▲ Rodlike particles near substrates exhibit critical Casimir torques controlled by the underlying chemical pattern of the surface.

▲ Changing the geometrical parameters of the pattern constitutes a crossover between different universality classes of boundary conditions

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Patterned surfaces and complex liquids

Discussion leader: S. Dietrich, MPI Institute for Intelligent Systems, Stuttgart, Germany

The discussion will address, but not be limited to, the following:

- Development of experimentally validated models for the wetting of ionic fluids, with a view to electro-wetting applications.
- Effect of surface patterning and topological defects on the wetting properties of liquid crystals, with a view to applications in the LCD industry.
- Interplay between additional length scales that characterise these fluids and the scale of the surface texture, and how this interplay may impact the wetting properties of such complex fluids.
- Role of thermal fluctuations and spatial correlations in determining wetting behavior.

POSTERS

Exotic liquid-vapor equilibria of patchy colloids

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In this contribution, I will present recent Monte Carlo simulation results [1, 2] for the phase diagrams of some lattice models of patchy colloids. The models represent colloidal particles whose surface contains two regions with different physicochemical properties. The first region (A) is defined by two interaction sites (patches), whereas the second region (B) comprises the remaining surface of the particle. The interactions between pairs of particles are short-ranged and depend on the regions of the spherical surfaces that are crossed by the vector that connects the centers of the two particles [3].

Within this interaction scheme, I will show how different choices of the parameters of the model lead to liquid-vapor phase diagrams with different topologies. More specifically, the following exotic cases will be considered: (a) Liquid-vapor equilibria with liquid phases behaving as empty liquids [1], and (b) Closed-loop liquid-vapor equilibria for one-component systems [2].

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Modeling liquid crystal lens with inhomogeneous polymer network in the cell bulk and at the cell walls

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We study a tunable-focus lens in which the key element is a gradient-polymer-stabilized liquid crystal (G-PSLC) structure [1]. It means that in the nematic liquid crystal cell there is a spatially inhomogeneous polymer network. The network is formed both in the cell bulk and at the cell walls. The later one modifies the liquid crystal director anchoring at cell substrates. This network creates an additional torque on the LC director forcing it to preserve planar orientation despite the applied voltage. The electro-optical response of the system to a uniform electric field is inhomogeneous but centrally symmetric. The refractive index profile is qualitatively similar to the director spatial distribution. The cell acts as a positive lens for extraordinary polarized light. By varying the applied voltage one can change the refractive index profile and hence control the focal length of the lens.

We have employed a recent theoretical model [2], to calculate the properties of this lens. Depending on the absorption of the light beam in the cell we study two separate model problems. The first model describes the case where the absorption of the light beam in the cell is weak and therefore the polymer network is formed mainly in the volume of nematic liquid crystal cell [3]. In the limiting case of strong light absorption a network may form close to one cell wall only, in which case the effect of the polymer network is only to modify boundary conditions at that wall [4].

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Non-equilibrium wetting by empty liquids

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We address the non-equilibrium adsorption of patchy colloids at planar attractive surfaces and characterize the obtained network fluids. By contrast to the equilibrium wetting films, the non-equilibrium films exhibit a fractal structure (gel) and the film density is always lower than the bulk equilibrium liquid density of the optimal network (zero pressure). The size dependence is well described by a power law with an exponent consistent with Diffusion Limited Aggregation and the density of the liquid film scales also with the diffusion constant as a power law with an exponent 0.23 ± 0.03 .

For a mixture of tri- and bivalent patchy colloids, the density of the liquid film is found to depend in a non-linear fashion on concentration ratio of species. At fixed size and diffusion constant the liquid film density initially increases with the concentration of bivalent colloids, peaks at a ratio ≈ 0.35 and then decreases. This contrasts to the equilibrium liquid film density of the optimal network that monotonically decreases, vanishing when the ratio approaches one. We provide an explanation for such difference based on the kinetics of adsorption.

The effect of walls on interacting boojum-colloids

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Colloidal particles dispersed in nematic liquid crystals (NLC), whose surface induces parallel alignment of the nematic molecules, induce the nucleation of surface defects called "boojums", which results in distortions in the nematic field with a quadrupolar symmetry. At short distances, surface defects start to interact directly and deviation from the quadrupolar interaction is observed. Recently, it has been shown that the core of boojums can exhibit some complex structure, and can undergo a structural transition when two colloidal particles are closely interacting. For close enough distances, and when the particles are aligned parallel to the far field director, the inner boojums will connect both particles, binding them together. This "bonded" configuration has been reported also in colloidal particles in cholesteric LC. Experiments have shown that the interaction between two spherical micron-sized particles dispersed in a NLC changes significantly when particles are close to a wall or confined in a narrow cell. Here we will present a numerical study on the stability of the bonded configuration, in the Landau-de Gennes framework. In particular, we will show how this configuration is affected by the presence of a wall, and under confinement.

Simulating immiscible two-phase flow and wetting by means of stochastic rotation dynamics (SRD) - from 2D to 3D

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We use the mesoscopic particle simulation method SRD to simulate immiscible two-phase flow on the pore and sub-pore scale. As an extension to the standard SRD method, we present a novel approach on implementing complex wettability on heterogeneous surfaces. Therefore, in a first step we simulate flow through a two-dimensional porous media where the substrate exhibits different spatial wetting correlations. We show how these wetting correlations influence the dynamics, in terms of percolation and residual saturation, through the porous media. As an outlook we present the extension of the SRD algorithm into the third dimension. Therewith it is possible to handle immiscible multi-phase flow in arbitrary geometries. Our preliminary results demonstrate the capability to address a variety of applications. This can be for instance flow through channels with different cross sections to study fluid dynamics on the sample scale. But also on the pore-scale SRD is a valuable tool to study for instance the formation of capillary bridges in an assembly of three or four spherical beads.

Resummed thermodynamic perturbation theory for central force associating potential. Multi-patch models

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A resummed thermodynamic perturbation theory for associating fluids with multiply bondable central force associating potential [1,2,3] is extended to account for the presence of several attractive sites. We consider a simple multi-patch model for associating fluids. The model is represented by the hard-sphere system with several circular attractive patches on the surface of each hard-sphere. Resummation is carried out to account for the blocking effects, i.e., when the bonding of a particle restricts (blocks) its ability to bond with other particles. Closed form analytical expressions for thermodynamical properties (Helmholtz free energy, pressure, internal energy, and chemical potential) of the model with arbitrary number of doubly bondable patches at all degrees of the blockage are presented. In the limiting case of total blockage, when the patches on the particles become only singly bondable, our theory reduces to Wertheims thermodynamic perturbation theory for polymerizing fluids [4]. To validate the accuracy of the theory we compare its predictions to exact values, for the thermodynamical properties of the system, as determined by Monte Carlo computer simulations. In addition we compare the fraction of multiply bonded particles with different number of patches and at different values of the density and temperature. Very good agreement between predictions of the theory, corrected for ring formation, and Monte Carlo computer simulation values was found in all cases studied.

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Supramolecular assembly of triblock rod – coil amphiphiles at liquid interfaces using classical density functional theory

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In the framework of Wertheim's perturbation theory we present a classical density functional theory for rod coil molecules with one rigid block and one or two flexible blocks. The theory is validated against molecular simulation for the case of an amphiphilic molecule in a selective pore. The theory is then applied to study the interfacial properties of the oil /water interface in the presence of triblock rod – coil amphiphiles (TBRCA's) consisting of a center rigid hydrophobic rod portion with flexible hydrophilic tails attached to each end. It is shown that TBRCA's preferentially adsorb to the interface in either a parallel or perpendicular orientation. The fraction of TBRCA's in each orientation can be manipulated by varying the length of the shortest flexible hydrophilic tail, length of the hydrophobic rod or the total number of TBRCA's at the interface.

**Mixed wettability on the mesoscopic scale:
Effect of wetting correlation length in porous media**

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In order to better understand the behavior of immiscible two phase flow through mixed wetting porous media, we have designed a series of experiments to test the effect of controlled heterogeneities (sub-grain) on a larger sample scale (order of 20,000 grains). The effective wettability of the heterogeneous samples is determined by measurement of the classical capillary pressure saturation curve. Here we present the effect of wetting correlation length within porous media from the sub-pore to lengths of half the sample height. Initial results indicate that average sample composition alone, cannot adequately describe the effective wettability of the sample, and thus the fluids behavior. Instead we observe that the size of the heterogeneity creates different environments and we obtain different fluid displacement profiles for different wetting correlation lengths. In particular, sub grain heterogeneity which impedes the formation of percolating wetting films impacts significantly of the two phase fluid behavior.

Inhomogeneous associating fluids - the liquid/vapour interface of patchy colloids

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In this work we investigate some aspects of the physics of associating fluids composed of patchy colloids - spherical particles which interact through a combination of centrally symmetrical repulsion and short-ranged directional attractive forces, arising from the presence of 'sticky spots' on the spheres' surfaces. Such systems were found to display very interesting phase behaviour, including re-entrant and pinched liquid/vapour coexistence curves, in the case when the spots decorating each colloid are not identical. We turn our attention to associating fluids placed in much less extensively studied inhomogeneous setups. Our model particles are hard spheres enhanced with three sticky spots each, out of which two are of type A and one of type B. Consequently, the colloids may form three types of bonds: AA (which lead to formation of linear chains), AB (producing Y-junctions), and BB (giving rise to X-junctions). We carry out a microscopic density functional theory (DFT) investigation of the properties of the liquid/vapour interface of the model fluid, and compare the results with an earlier analysis, which applied a Landau-type theory.

Photorefractivity and two-beam energy exchange in a hybrid organic-inorganic cell containing ferroelectric nano-particles

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Recently we have developed a procedure to harvest 9nm sized ferroelectric nano-particles of BaTiO₃ [1-3]. These nanoparticles not only possess a spontaneous polarization, but the polarization is several times higher than that of the bulk material. Doping liquid crystals with ferroelectric nano-particles significantly changes the dielectric and optical properties of the suspension. In this work we develop a theory to describe the experimentally observed energy gain enhancement when two light beams intersect in hybrid photorefractive-liquid crystal system. The hybrid system consists of a nematic liquid crystal (LC) layer doped with ferroelectric nano-particles and placed between two photorefractive windows. A periodic space-charge field is induced by the interfering light beams in the photorefractive windows. The space-charge electric field penetrates into the LC layer, interacting with the nematic director and ferroelectric nano-particles giving rise to a periodic modulation of the colloid refractive index. LC flexoelectricity and nano-particles spontaneous polarization are the principal players driving rise to the periodic modulation of the colloid refractive index. Periodic modulation of the director and nano-particles optical axis creates two spatially shifted refractive index diffraction gratings. Each light beam diffracts from the induced gratings, leading to the energy gain and loss within each beam. The LC optics is described in the Bragg regime using coupled wave theory and small beam gain coefficient is calculated.

Our theoretical modeling is compared with results of the experimental study of hybrid cells filled with LC TL205 doped with BaTiO₃ nano-particles [4]. Experimentally the energy gain is maximal at much lower grating spacing than it was predicted early by a naive theory. Besides, an addition of nano-particles to TL205 results in the sign change of the gain coefficient when the grating spacing and nanoparticles concentration increase. Supposing the magnitude of the gratings to be a nonlinear function of space-charge field we obtain a good agreement between our theoretical modeling and the experimental data. We provide semi-quantitative arguments to justify this non-linearity in terms of electric-field-induced local phase separation of the LC colloid.

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Effect of ions on confined near-critical binary aqueous mixture

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Near-critical binary mixtures containing ions and confined between two charged and selective surfaces are studied within a Landau-Ginzburg theory extended to include electrostatic interactions. The obtained charge density profiles and the effective interactions between the confining surfaces show that close to the critical point of the binary solvent, the preferential solubility of ions for one of the solvent components leads to the modification of the charge density profiles in respect to the ones obtained from the Debye-Hückel theory. As a result, when the bulk correlation length ξ of a solvent is much larger than the Debye screening length κ^{-1} the electrostatic contribution to the effective potential between the charged surfaces can exhibit an attractive well. We show a quantitative agreement between the obtained results and the recent experiment reporting the effective forces acting between a substrate and a spherical colloidal particle immersed in the near-critical water-lutidine mixture [Nature **451**, 172 (2008)]. Moreover, for the range of $\kappa\xi \leq 1$ the results show an unexpected attraction between the hydrophilic and the hydrophobic surface for some range of $\kappa\xi$, in agreement with the recent experiment [Nellen *et.al.*, Soft Matter **7**, 5360 (2011)].

Nanofluidics: Dynamics of thin films and nano-droplets

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Fluids on the nanoscale behave qualitatively different from macroscopic systems. This becomes particularly evident if a free liquid-liquid or liquid-vapor interface is close to a solid surface such as in the case of nanodrops or ultrathin films. Hydrodynamic slip, thermal fluctuations, the molecular structure of the fluid, and the range of the intermolecular interactions are important for the structure and the dynamics of such open nanofluidic systems.

Here we focus on a top-down approach to the theoretical description of fluids on the nanoscale: mesoscopically augmented hydrodynamic equations. We discuss their application to the dynamics of dewetting on homogeneous substrates as well as on the dynamics of nanpdroplets and rivulets on topographically or chemically structured substrates.

Structure and thermodynamics of the dipolar hard-sphere fluid at low temperatures and densities

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Through extensive state-of-art numerical simulations, we study the behavior of the dipolar hard sphere model at low temperatures and low densities, shedding light on a region of the phase diagram where a topological phase transition has long been thought to occur. Despite a lack of phase separation, we show that the system exhibits remarkable and unusual behaviors like a very low density percolation locus and a stabilization of rings over chains at extremely low densities. This unexpected abundance of rings comes from a delicate balance between the lower ring energy and the end-to-end chain entropy, and hints at a possible mechanism for the suppression of the gas-liquid phase separation. Our results open the possibility for refined theoretical approaches which, in addition to the previously encompassed chain and branched geometries, must also include the significant contribution arising from ring formation.

Advancing and receding modes on patterned substrates

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Contact angle hysteresis is a relevant feature necessary to characterize wetting on heterogeneous surfaces. Despite the large amount of studies in the recent years, quantitative predictions only based on the geometric and chemical features are still missing. A detailed simulation of the liquid interface allows us to calculate stable morphologies on regular patterns of square arrays of pillars either with square and circular cross section. Both hydrophilic and hydrophobic substrates are considered. The apparent contact angle is used as a control parameter, and its variation leads to several topological changes of the liquid interface. Non stable configurations define advancing (receding) angles of the whole interface. Depending on the last stable topology, different modes are found. Varying the density of pillars sharp, variations of advancing angles are found. Similarities and differences respect to the shape of the pillars are defined in regions of the space of parameters. This study represents a step towards a general description of motion on a rough surface and helps in designing surfaces with well defined properties.

The structure of boojums on nematic colloids

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Topological defects play a key role in the interaction of colloidal particles in liquid crystals. They appear as a consequence of broken orientational order, and their distribution around the colloidal particles determines the symmetry of long-range interactions. Colloidal particles induce surface alignment of the nematic molecules. When the nematic is aligned parallel to two surface topological defects, known as boojums, are nucleated at opposite ends. In two-dimensional systems, boojums are always point-like. Here we show that, in three-dimensional systems, these defects acquire a rather complex structure that depends on the combination of surface potential, size of the colloidal particle, temperature, and the liquid crystal elastic anisotropy.

Magneto-optical effects in twisted nematic liquid crystals doped with ferromagnetic particles

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In recent years much attention has been paid to study of liquid crystal based metamaterials [1,2]. In these materials nano particles of different nature (metallic, ferroelectric, ferromagnetic) and shape (rods, wires, and spheres) are dispersed in liquid crystalline host materials. Recent theoretical and simulation studies have revealed new features of nematic systems containing ferromagnetic particles (ferronematics). In particular, inverse Frederiks effect [3] was predicted. Nematic and magnetic director reorientation and optical response of a $\pi/2$ -twisted ferronematic cell to the in-plane weak external magnetic field was investigated in [4].

In this work we report a theoretical study of nematic and magnetic director reorientation and optical response in a $\pi/2$ -twisted ferronematic cell, subject to a weak (< 50 Oe) external magnetic field *perpendicular* to the cell surfaces. One cell surface is strongly anchored and another is weakly anchored. Normally incident light passes through polarizers whose relative angle can vary.

The ferroparticle magnetic order and concentration couple strongly with the nematic director. The initial director configuration is in the cell plane. Increasing magnetic field causes this configuration to reorient out-of-plane.

The structural transition (Fig.1) may be continuous or first-order, depending on system parameters. This reorientation is coupled to nematic director reorientation and colloidal density inhomogeneity, resulting in optical heterogeneity of the nematic across the cell. The reflected and transmitted light intensities vary significantly and non-monotonically as a function of field (Fig.2).

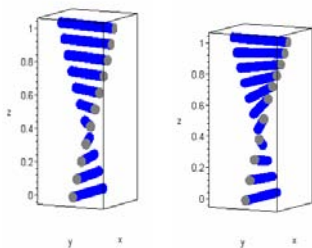


Fig. 1. Maximal deviation of the nematic director out-of plane angle vs. applied magnetic field.

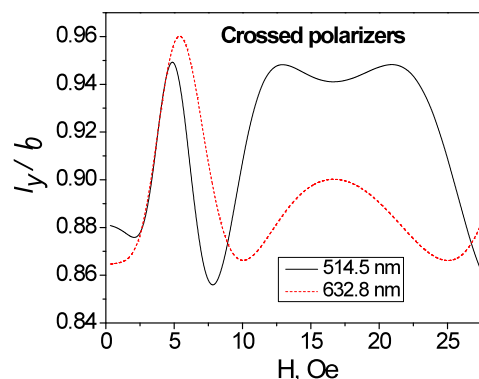


Fig. 2. Relative intensity of the transmitted light vs. applied magnetic field.

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Abstract Book

PROGRAMME

	Wednesday, October 10	Thursday, October 11	Friday, October 12
8:45 - 9:00	<i>Opening remarks</i>		
9:00 - 10:00	C. Cottin-Bizonne	P. Poulin	D. Aarts
10:00 - 10:30	M. Popescu	O. Gang	A. Parry
10:30 - 11:00	<i>Coffee Break</i>		
11:00 - 11:30	M. Brinkmann	A. Law	J.M. Romero-Enrique
11:30 - 12:00		A. Maciolek	V. Reshetnyak
12:00 - 12:30	A. Checco	N. Bernardino	M. Blow
12:30 - 14:00	<i>Lunch Break</i>		
14:00 - 15:00	Discussion	F. Sciortino	J. Yeomans
15:00 - 15:30		D. de las Heras	M. Tröndle
15:30 - 16:00		<i>Coffee Break</i>	
16:00 - 16:30	<i>Coffee Break</i>	M.M. Telo da Gama	Discussion
16:30 - 17:30	F. Martinez-Veracoechea	Discussion	
17:30 - 18:00	A. Tkachenko		
18:00 - 18:30	B. Ocko		

20:00 - 22:00

Workshop dinner

Sponsors:

