Poster abstracts

The abstracts are organised by topics: Active Soft Matter (AC1-49), Arrested Soft Matter (AR1-17), Colloidal Soft Matter (CO1-52), Interfacial Soft Matter (IN1-45), Living Soft Matter (LI1-16), Making & Measuring Soft Matter (MA1-9), Polymeric Soft Matter (PO1-41), Processing & Stressed Soft Matter (PR1-17) and Self Assembled Soft Matter (SA1-36).

AC1 Bacterial Microswimmers in Colloidal Liquid Crystals

ALEXANDER, Lachlan C. (University of Bordeaux), GRELET, Eric (University of Bordeaux); AARTS, Dirk (University of Oxford)

Simple active systems, at the colloidal scale, become very good tools to understanding complex interactions in nature. There are many biological phenomena, which involve microswimmers, that are yet to be explained or broken down into basic components. These include those where microswimmers exist within dense frameworks, such as in biofilms or infected tissues. There have been only a few studies to date which aim to tackle the behaviours of active particles in a dense background. In our study we investigate aspect of the interaction between microswimmers and an intrinsically ordered liquid crystal matrix [1]. We wish to explore the effect of bringing the mesogens of the liquid crystal to within the order of magnitude of the size of the microswimmers. To do this we use a colloidal liquid crystal formed by the filamentous fd virus. This enables us to look into a wide range of liquid crystalline behaviours expressed by fd virus suspensions with varying particle concentrations. We look into how the increased size of the liquid crystalline particles affects *Bacillus subtilis* in the nematic and smectic phases. We pay particular attention to the smectic ordering potential and how it couples with the activity of the microswimmers and adds to their motion.

[1] Command of active matter by topological defects and patterns. Peng, Chenhui and Turiv, Taras and Guo, Yubing and Wei, Qi-Huo and Lavrentovich, Oleg D. Science 18 Nov 2016, Vol. 354, Issue 6314, pp. 882-885. DOI: 10.1126/science.aah6936

AC2 Reconfigurable thermo-responsive active colloids

ALVAREZ, Laura (ETH Zurich), FERNANDEZ-RODRIGUEZ, Miguel Angel (ETH Zurich), ISA Lucio (ETH Zurich)

Active colloids, the synthetic analog of biological microswimmers, can harvest energy from a uniform source and convert it into propulsion thanks to an asymmetry in their shape or composition [1]. However, they lack inherent sensing and adaptive capabilities as, e.g. chemo-, photo- and magnetotactic behavior exhibited by bacteria [2]. Therefore, producing active colloids that can adapt their shape, velocity, and reorientation to environmental stimuli remains an open challenge. In this work, we present a new generation of adaptive active colloids combining thermo-responsive microgels (PNiPam-co-AAc) with fluorescent microparticles fabricated via sequential capillary assembly (sCAPA). These active colloids are powered by AC electric fields and can reconfigure as a result of a local temperature variation causing a change of the microgel size. We explore the dynamics of different particle geometries: dumbbells, triangles, and L-shapes. In all cases, the propulsion speed and the characteristic reorientation time change when the microgels shrink due to a local temperature increase caused by light absorption of the fluorescent particles. As a consequence, the persistence of the active particle trajectories can be modulated by varying the illumination. The feedback between illumination, particle shape and dynamics is also explored by imposing simple light patterns. The fabrication of these new reconfigurable active colloids constitutes another step in the pursuit of autonomous active microsystems.

[1] C. Bechinger, et.al., Revi. Mod. Phys, 88, 045006-045056 (2016).

[2] K. Son, et.al. Nature Reviews, 13, 761-775 (2015).

AC3 Illumination-induced motion of Janus particle in binary mixtures

ARAKI, Takeaki (Kyoto University), MACIOLEK, Anna (Max Planck Institute for Intelligent Systems)

Janus particles, which have heterogeneous surface properties, are often employed as artificial self-propelled systems. For example, the self-propelled motions are modelled by asymmetric nanoparticles partially coated with platinum. The catalytic decomposition of hydrogen peroxide, which occurs selectively on the Pt-surface, drives the nanoparticles. Interfacial phoretic effects are another possible mechanism of micro-swimmers. It was demonstrated that a Janus particle can create an asymmetric temperature gradient around it in a defocused laser beam. Bechinger and his coworkers studied Janus particles immersed in binary mixture of lower critical solution temperature. The half hemisphere of the particle is covered by a metal or carbon. Under a light illumination, the temperature is increased locally around the covered surface, and then, the concentration field of the binary mixture becomes heterogeneous around the particle. They observed the particle move spontaneously along the orientation of the Janus particle. In this study, we consider such propelled motions of the Janus particle in binary mixtures. We employ fluid particle dynamics simulation, in which each spherical particle is mapped with a sigmoid function on a lattice space. We numerically solve the dynamics of the particle motion, the concentration field, the temperature field and the hydrodynamic flow. We assume that the head side of the particle is selectively heated by an external source. We found that the concentration field around the head becomes remarkably heterogeneous under the illumination. The concentration gradient causes the hydrodynamic flow and this flow tends to push the particle along the particle orientation. Our simulations indicate this particle motion is due to the Marangoni effect of the interface tension under the temperature gradient, not due to the thermos- or diffusio-phoretic effects. The speed and the direction of the particle motion depends not only on the heating rate, but also on the wettability. When the particle surface is homogeneously neutral in the wettability, the particle does not move under a weaker illumination than a threshold. Above the threshold, the particle moves forward and its speed is increased with the heating rate. When the particle wettability is asymmetric and the head side prefers one of the solvent components more than the tail side, on the other hand, the particle can move even under a weak illumination. We also found the inversion of the motion direction with the heating rate when the tail side has a larger wettability. The particle moves backward under a weak illumination, while it moves forward under a strong illumination.

AC4 A systematic Markovian approximation for active particles

BAEK, Yongjoo (DAMTP, University of Cambridge)

Self-propelled particles form a class of nonequilibrium systems with a constant injection of energy on a microscopic scale. Given sufficient time-scale separation, one can model such particles using the Langevin dynamics with an instantaneous damping force and a Gaussian colored noise with rapidly decaying correlations. To make the model analytically tractable, previous studies have proposed various Markovian approximation schemes which replace the colored noise with a multiplicative Gaussian white noise; however, these approaches are not systematic and may restore equilibrium-like steady-state behaviors, failing to capture the nonequilibrium aspects of the steady state. In this talk, I present a systematic Markovian approximation, which yields a Langevin equation with a multiplicative non-Gaussian white noise. The nonzero skewness of the noise is shown to be essential for correctly predicting the evolution of the probability distribution function. The approach provides a convenient and reliable method for predicting nonequilibrium currents, forces, and first-passage time statistics associated with self-propelled particles.

AC5 New Energy Generator by Trampolining Elastic Gel (NEGTEG)

BEN XU (Northumbria University at Newcastle); Sridhar, Sreepathy (Northumbria University); Liu, Yingzhi (HIT); Li, Yifan (Northumbria University); Lv, Haibao (HIT); Wang, Steven (Newcastle University)

In this research, we demonstrate an emerging thermo-electric generating technology based on Leidenfrost effect induced trampolining of elastic gel on hot surface1, which occurred under a coupling effect from the elasticity of gel and Leidenfrost effect2. Knowledgeable by the Leidenfrost effect ? a water based system can be levitated by its own vapour layer on an extremely hot surface can be tuned by modulating the vapour layer arising from increased heat flux from underlying highly superheated substrates. The thermal energy was transferred into electric energy through a levitation activated mechanical motion, supported by a self-constructed piezoelectric-hydrogel system. The studies were carried out with different material elasticity (0.5kPa ? 100kPa), size (6mm ? 20mm), surface temperatures and surfaces. After careful optimization of the selected gel spheres, we elaborately studied other factors such as mass loss, impact dynamics, energy generation, etc. In this study, the maximum surface temperature was limited to 350C. Up to this temperature, the system can bounce by retaining its shape and water content for extended time (Fig 1). We achieved a conversion unit to produce an optimum 3V and expected to get higher output (¿ 30V) by integrating a number of same units. Knowledgeable by the Leidenfrost effect ? a water based system can be levitated by its own vapour layer on an extremely hot surface can be tuned by modulating the vapour layer arising from increased heat flux from underlying highly superheated substrates. This finding opens a window to create an energy-harvesting device that can generate electrical power from thermal sources and offer a potential solution for those regions with rich geo-thermal resources to acquire electric energy, such as Iceland or volcanic islands.

AC6 A phase diagram for an active nematic confined to a spherical shell

BROWN, Aidan (University of Edinburgh)

An ‘active nematic’ is a nematic liquid crystal endowed with self-generated motion. Recent experiments [1] have studied the behaviour of an active nematic film made from microtubules and molecular motors confined to the surface of a spherical vesicle. The spherical topology produces four +1/2 nematic defects, which then become self-propelled due to the activity. Combined with an elastic repulsion between the defects, this leads to an intricately coordinated dance in which the defects periodically oscillate between tetrahedral and planar configurations. Several groups have modeled this defect motion, both at the molecular level [2], and in terms of a ‘point-particle’ model for the defects [1, 3]. Interestingly, these approaches predict qualitatively different types of oscillation, with the molecular-level study agreeing more closely with experiment.

Here, I will show that these differences can be resolved by modifying the existing point-particle models to properly take into account the spherical geometry. Further, by varying the parameters of defect speed, orientational and translational stiffness, I find that this modified model exhibits other qualitatively distinct, oscillatory states, which have not yet been observed experimentally. Intriguingly, in one region of parameter space the defect orbit itself precesses, and often multiple, metastable states can coexist. I will show that these features can be understand via linear stability calculations, and discuss the implication of these results for future experiments on active nematics.

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[2] Zhang, R., et al., (2016) Dynamic structure of active nematic shells, Nature Communications 7, 13483

[3] Khoromskaia, D., and Alexander, G. P., (2017) Vortex formation and dynamics of defects in active nematic shells, New Journal of Physics 19, 103043

AC7 Active nematics in channels

Chandragiri Santhan (Indian Institute of Technology Madras); Doostmohammadi, Amin (University of Oxford); Yeomans, Julia (University of Oxford); Thampi P, Sumesh (IIT Madras)

Active nematics is a promising model system for active matter like dense suspensions of microtubule bundles with kinesin motors, colonies of bacteria like E.coli or human cells. Recent experiments of active matter in simple geometries show that confinement plays a major role in determining the type of active flow. We use continuum simulations to study the dynamics of confined active nematics. Our studies show that the width of the channel and flow aligning parameter are key parameters in determining the type of active flow in two dimensions. In addition, aspect ratio of the channel is a key parameter in three dimensional confinements. Previous studies assume the presence of a free energy in determining the orientational order in active nematics. However such ordering mechanisms observed in passive liquid crystals are probably not present in biological systems. Therefore, we study active nematics above and below the isotropic-nematic transition temperature and show that the presence of activity is sufficient to generate orientational order in active nematics. Moreover, the strength of orientational ordering generated by passive and active mechanisms play a major role in determining the type of flow obtained.

AC8 Circle microswimmers in crowded media. Limit of ideal trajectories and the influence of noise.

CHEPIZHKO, Oleksandr (Institute for Theoretical Physics, University of Innsbruck, Austria); FRANOSCH, Thomas (Institute for Theoretical Physics, University of Innsbruck, Austria)

Itn nature microswimmers move in crowded environments and their transport properties strongly depend on the particular rules of interaction with obstacles. Here, we study a model of a circular microswimmer that moves in circles in freely accessible space and follows the surface of obstacles for a certain time after collision. We begin by considering the case of an ideal microswimmer that moves in perfect circles [1]. Depending on the model parameters such as the orbit radius and the density of the obstacles, the microswimmer can perform diffusive motion or be localized. One of the localizations originates from a percolation transition of the underlying void space. Another localization is connected to the low-density limit when the microswimmer can not meander from one isolated obstacle cluster to another. We study in detail the crowding enhancement of the diffusivity, caused by the wall-following mechanism. We rationalize the transitions from the localized states to the diffusive state as a dynamic critical phenomenon. Next, an angular noise term is added to the direction of motion between interactions with obstacles. This smears the phase diagram, as now long-range transport can happen at any density of obstacles. We investigate how the quality factor, number of full circles in one diffusion time, influences the diffusivity.

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AC9 Biological mixing across dimensions

Dmitri O. Pushkin (University of York)

Suspensions of microscopic swimmers turn out to be efficient stirrers – this fact has important ecological and technological consequences. Past theoretical work has distinguished two distinct mechanisms of biomixing in dilute suspensions of swimmers: the one due to entrainment of fluid particles in the immediate neighbourhood of a swimmer, and the one due to far-field flows created by multiple swimmers. The relative importance of these mechanisms has been studied theoretically and experimentally for three-dimensional (unbounded) suspensions over short and long time scales of the experiment. The arising picture is well-understood, if nuanced. By contrast, the nature and relative importance of the stirring mechanisms in active suspensions confined by parallel walls is not well-understood. In this talk, we survey the results of older and more recent experiments to highlight the surprising properties of biomixing under varying degrees of confinement. We present a semi-analytical mathematical model allowing to understand and classify the varieties of observed transport processes. In particular, we show that stirring under confinement may give rise to qualitatively different types of stirring, governed by the boundary conditions and the degree of confinement. For each case, we present a simple scaling law describing the ensuing effective diffusivity.

AC10 Acoustic propulsion of metallic nano-cylinders: contribution of the local vertical acceleration

DUMY, Gabriel (PMMH Laboratory, ESPCI Paris); AIDER, Jean-Luc; HOYOS, Mauricio

Acoustic manipulation of microscopic objects can be performed using ultrasonic standing wave resonators and is called acoustophoresis. Provided that the wavelength of the acoustic field (generated in this case by a piezoelectric transducer) and that one of the cavity dimensions verify ? = 2h, an ultrasonic stationary wave can be generated between two opposite walls of said cavity. This field can have two effects on the cavity components: on scattering particles it will exert a net body force, and it will transfer momentum to the fluid filling the cavity resulting in a streaming flow. Thus, a suspension of microscopic objects submitted to such a field will see its constituents driven towards the pressure nodes (or antinodes depending on particles properties), where they can be trapped. The typical size of the objects that can be moved by acoustophoresis ranges from 500 nm to several tens of microns.

A surprising finding in ultrasonic manipulation of micron-sized objects is the auto-propulsion of metallic nano-cylinders when trapped in such a field: instead of aggregating like spherical particles, they start to swim while being confined in the pressure node of the acoustic field. The phenomenon has first been described with nano-cylinders made of gold, with a 200 nm diameter, and 1 μm length. Motion ranging from straight lines to circular trajectories is observed. It is an intriguing phenomenon, since these quite small particles can propel up to hundredth of sizes per seconds, while within a $R_e \simeq 10^{-4}$ flow. In addition, these particles can organize themselves in chains hundredth of microns long because of their rotation, showing interesting self-assembling properties. Moreover, the power levels used here are on par with medical echography devices, and these nanorods have proven to be active even in cells, showing interesting potential for bio-oriented applications.

Investigations have been conducted in the presented work on the contribution of the local acceleration of the gravity field on the orientation of the nano-cylinders, and its potential role in the propulsion of these objects. Indeed, the aggregating position differs from the geometrical pressure node thanks to buoyant forces, and these ones are non-negligible for metallic particles. We compared laboratory and microgravity experiments, to correlate between the vertical position of the aggregate and the propulsion speed of the swimmers. We observed a different behavior of the cylinders in each case, and this may be a clue of the role played by the transverse component of the acoustic forces to the propulsion of these objects.

AC11 Activity-Induced Breakup of Colloidal Aggregates

GRIFFITHS, Sam (The University of Edinburgh); KOUMAKIS, Nick (The University of Edinburgh); VISSERS, Teun (The University of Edinburgh); BROWN, Aidan (The University of Edinburgh); POON, Wilson (The University of Edinburgh)

We study experimentally the effect of doping a phase separating two-dimensional system of colloids and polymers with a low concentration of active particles in the form of motile Escherichia coli bacteria. We find that the active dopants transform the crystal-fluid region of the phase diagram of the passive system into a region of micro-phase separation, where individual two-dimensional rafts of colloidal crystals coexist with a colloidal gas phase. The cluster size distribution can be ‘tuned’ by the polymer and bacterial concentrations.

AC12 How active forces influence nonequilibrium glass transitions

Grzegorz Szamel (Department of Chemistry, Colorado State University)

Physical intuition suggests that increasing departure from equilibrium due to active forces fluidifies a glassy system. We falsify this belief by devising a model of self-propelled particles where increasing departure from equilibrium can both enhance or depress glassy dynamics, depending on the chosen state point. We analyze a number of static and dynamic observables and suggest that the location of the nonequilibrium glass transition is primarily controlled by the evolution of two-point static density correlations due to active forces. The dependence of the density correlations on the active forces varies non-trivially with the details of the system, and is difficult to predict theoretically. Our results emphasize the need to develop an accurate liquid state theory for nonequilibrium systems.

AC13 Phase coexistence of active Brownian particles: Anything for a quiet life

HERMANN, Sophie (Universitt Bayreuth); KRINNINGER, Philip (Universitt Bayreuth); DE LAS HERAS, Daniel (Universitt Bayreuth); SCHMIDT, Matthias (Universitt Bayreuth)

We investigate motility-induced phase separation of active Brownian particles, which are modeled as purely repulsive soft spheres that move due to a constant swim force with freely diffusing orientation. We develop from first principles an analytical theory for nonequilibrium phase coexistence and interfacial structure. Theoretical predictions are validated against Brownian dynamics computer simulations. We show that the internal one-body force field has four nonequilibrium contributions: (i) isotropic drag and (ii) interfacial drag forces against the forward motion, (iii) a superadiabatic spherical pressure gradient and (iv) the quiet life gradient force. The intrinsic spherical pressure is balanced by the swim pressure, which arises from the polarization of the free interface. The quiet life force opposes the adiabatic force, which is due to the inhomogeneous density distribution. The balance of quiet life and adiabatic forces determines bulk coexistence via equality of two bulk state functions, which are independent of interfacial contributions. The internal force fields are kinematic functionals which depend on density and current, but are independent of external and swim forces, consistent with power functional theory. The phase transition originates from nonequilibrium repulsion, with the agile gas being more repulsive than the quiet liquid.

AC14 Shear viscosity of active enzyme solutions

HOSAKA, Yuto (Tokyo Metropolitan University); ANDELMAN, David (Tel Aviv University); KOMURA, Shigeyuki (Tokyo Metropolitan University)

Active proteins play important roles in catalyzing chemical reactions with the supply of a substrate such as ATP. Recently, non-equilibrium effects induced by these proteins have attracted many interests and have been studied both theoretically and experimentally. For example, a force dipole model was employed to derive the diffusion coefficient of a passive object in physiological environments such as a cytoplasm and a surrounding biomembrane (Mikhailov and Kapral, 2015).

As one of the active systems with ATP-driven proteins, we chose a dilute suspension of active elastic dumbbells under steady shear flow. Here active dumbbells represent catalytic enzymes, and we derive the active enzyme viscosity η_{a} by using the above force dipole model.

The separation between the dumbbell beads is governed by the Langevin equation where the elastic energy $U(r, s)$, the thermal noise, and the shear flow are considered. Here, $U(r, s)$ is the state-dependent term which represents the turnover cycle of the actual enzyme.

By analytically solving the constitutive equation, we find that η_{a} presents both decreasing and increasing behaviors as the substrate concentration is increased, depending on the physical properties of the binding substrate. For a substrate larger than the enzyme, we see that η_{E} behaves as if no substrate were present because it does not affect the size of the enzyme.

AC15 Experiencing the Force: giant photomechanical transduction in a thermophoretic quantum dot suspension

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Since the historical experiments of Crookes, the direct manipulation of matter by light has been both a considerable challenge and a cause for intense scientific debate. Here we show that irradiation with a 1.5 W laser beam allows to displace a macroscopic vial containing a lead sulfide nanoparticle solution over centimeter-scale distances. Cantilever-based force measurements show that the movement is due to millisecond long and a few mN high force spikes, which are accompanied by a sound emission, and that spikes are triggered only above a critical laser power. Moreover, ultrafast imaging reveals that the force spikes are accompanied by the explosive growth of a bubble in the solution. We propose a mechanism accounting for the observed behaviour, based on negative thermophoresis of the lead sulfide particles, and a Jeans 'gravitational' instability of the nanoparticle cloud. The phenomenon at stake would be the first experimental observation of such an instability. Our experiments thus demonstrate a new type of laser propulsion, and a remarkable macroscopic consequence of negative thermophoresis.

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AC16 The swimming modes of barnacle cypris larvae

Kei Kikuchi (Akita Prefectural University); Yukitaka Ishimoto(Akita Prefectural University); Keju Okano (Akita Prefectural University); Stephanie Nix (Akita Prefectural University)

Barnacle is a type of crustacean with two distinct larval stages, the nauplius and cypris stages. Cypris larvae of 200 to 300 mm in length are on a mission to find a favourable surface to settle and cement themselves on. Because this mission seems to be so easily and successfully fulfilled, barnacle is known as a major source of biofouling for ships and power plants while it is also a food resource on the other hand. As well as from these environmental and agricultural points of view, a better understanding and elucidation of the barnacle navigation system have been anticipated: why they settle where, and how they navigate themselves in sea. Being founded by Sir Charles Darwin, barnacle has been studied for centuries. Many ecological features of barnacles have been revealed, and some of cypris motion have been shown. For example, cyprids are strongly attracted by adult pheromones and infrared light from adult outer test. However, little is known about the mechanism of their gregarious settlement on an adult-free surface, cypris swimming modes, and their mechanical details. In order to elucidate the barnacle cypris navigation system, we tracked and quantified barnacle larvae swimming in a pseudo-two-dimensional chamber and analysed characteristics of their swimming motion. We set up the chamber by a pair of parallel acrylic boards with a rubber spacer between them, and visualise their motion by casting a sheet laser parallel to the board. We investigated the Rhizocephalan barnacle. The motion was captured by a high-speed camera with a framerate of 250 fps and processed with image manipulating software. With the processed data, we investigated swimming patterns, velocity cycle, velocity autocorrelation and FFT of velocity autocorrelation. Finally, we found that a cypris larva shows a cyclic movement: it strokes six legs twice in a cycle. We further confirmed four swimming patterns (a): continuous swimming, (b) intermittent swimming, (c) turning, and (d)sinking. The mode (b) is basically the mode (a) with repeated rests. The average maximum speed were about 40 mm/s in (a) and (b), while it was about 20 mm/s in (c). The velocity cycle and FFT analysis show basically different peaks in frequency distribution in each mode. Velocity autocorrelation shows that periodicity in the correlation exhibits individual differences of the same species. Their collective motion will also be mentioned in the end.

AC17 Simple swimmers reverse direction near a surface

Kuron, Michael (Universität Stuttgart); Stärk, Philipp (Universität Stuttgart); Holm, Christian (Universität Stuttgart); de Graaf, Joost (Universiteit Utrecht)

The motion of a microswimmer can change substantially in the presence of a surface. For example, sperm move in circular trajectories near a wall [1], paramecia swim along sinusoidal trajectories through a tube [2], and chemical swimmers can orbit around spherical obstacles [3]. In this work, we investigate the behavior of a spherical squirmer, a model microswimmer, interacting with spherical objects and we explore the flat wall limit. We report three distinct behaviors — orbiting/sliding, scattering, and hovering — depending on the surface curvature and the strength of the squirmer's hydrodynamic dipole moment. Interestingly, we also observe cases where the squirmer orbits/slides along a surface in a direction opposite to the one it moves in bulk. This effect is present both in our far-field numerical calculations and in our lattice Boltzmann simulations, which accurately account for the near-field flow. We show that the backward motion is caused by the hydrodynamic quadrupole in the squirmer's flow field, which explains why this motion was not observed in previous studies that truncated the hydrodynamic expansion at lower order [4]. We make quantitative predictions about the transition between scattering and orbiting and argue the importance of accounting for higher-order hydrodynamic moments associated with finite swimmer size. Our results further underpin the need to perform bulk experiments to accurately assess the effect of varying environmental parameters.

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AC18 Swimmers in Smectics

LAKEY, Christopher (University of Warwick); TURNER, Matthew (University of Warwick)

Continuum models describe the interactions between colliods embedded in smectic liquid crystals [1-3]. The presence of embedded particles, of diameter comparable to the smectic layer spacing, results in a distortion of the smectic ordering. We consider a system of self-propelling colloidal particles ('swimmers') in a smectic liquid crystal. These swimmers are confined between the smetic layers, but interact with swimmers in other layers via the distortions that they induce in the smectic ordering. We find that the motion of these swimmers is then controlled by a combination of their own motility and the forces that they experience from the smectic mediated interaction potential, giving rise to rich dynamical behaviour.

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AC19 Consensus vs polarization: Collective behavior of active particles with selective interactions

LOBASKIN, Vladimir (University College Dublin); Maksym Romenskyy; Thomas Ihle

We study the orientational ordering in systems of self-propelled particles with selective interactions. To introduce the selectivity we augment the standard Vicsek model with a bounded-confidence collision rule: a given particle only aligns to neighbors who have directions quite similar to its own. Neighbors whose directions deviate more than a fixed restriction angle α are ignored. The collective dynamics of this system is studied by agent-based simulations and kinetic mean-field theory in the hydrodynamic limit [1]. We show that upon decreasing the restriction angle and the noise amplitude the system develops an orientationally ordered polar state. The transition between the ordered and disordred states can be either continuous or discontinuous, which controlled by the formation of density bands. At very small interaction angles, the polar ordered phase becomes unstable with respect to the bipolar phase. We derive analytical expressions for the dependence of the threshold noise on the restriction angle. We calculate the critical noise, at which the disordered state bifurcates to the bipolar state, and find that it is always smaller than the threshold noise for the transition from disorder to polar order. We generalize our results to systems that show fragmentation into more than two groups and obtain scaling laws for the transition lines. Finally, we discuss the similarity of this interaction model to bounded confidence models in social simulation and demonstrate an application of it to modelling opinion dynamics [2].

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AC20 Current-mediated synchronization of a pair of beating non-identical flagella

MACIOLEK, Anna (Max-Planck-Institute for Intelligent Systems); DOTSENKO, Viktor (Sorbonne Université), OSHANIN, Gleb (Sorbonne Université), VASILYEV, Oleg (MPI IS Stuttgart), Dietrich, S (MPI IS Stuttgart)

The basic phenomenology of the experimentally observed stochastic phase-locking of beating flagella of a biflagellate alga is captured well by a minimal model involving two noisy Kuramoto oscillators with the noise amplitudes depending on the flagella lengths. We address the conceptually important question which kind of synchrony occurs if the two flagella have different lengths such that the noises acting on each of them have different amplitudes. Within a minimal model, too, we show that in this case a different kind of synchrony emerges, mediated by a current-carrying steady state.

AC21 Coarsening phenomena around hot Janus colloid

MACIOLEK, Anna (Max-Planck-Institute for Intelligent Systems, Stuttgart); ROY, Sutapa (MPI IS, Stuttgart), GOMEZ-SOLANO, Juan Ruben (National Autonomous University of Mexico), and DIETRICH S. (MPI IS, Stuttgart)

Laser illuminating a Janus colloid which is suspended in a near-critical binary solvent leads to the formation of the concentration gradient and coarsening patterns around the colloid. Using analytical theory and numerical simulations, we investigate the non-equilibrium dynamics of this phenomenon under the influence of a time-dependent temperature gradient. Our predictions are also confirmed by experiments with gold cap Janus particles immersed in PnP-water binary liquid mixture. Time-dependent properties of the coarsening patterns for various surface adsorption properties of the Janus colloid are analyzed. We also observe that the particle starts to move much before the stationary state is achieved.

AC22 Rheo-imaging of a swimming bacterial suspension: effect of system-size

MARTINEZ, Vincent (School of Physics & Astronomy, The University of Edinburgh); CLÉMENT, Eric (ESPCI); Arlt, Jochen (University of Edinburgh); DOUARCHE, Carine (University Paris-Sud); DAWSON, Angela (University of Edinburgh); SCHWARZ-LINEK, Jana (University of Edinburgh); CREPPY, Adama (University Paris-Sud); AURADOU, Harold (University Paris-Sud); MOROZOV, Alexander (University of Edinburgh); POON, Wilson (University of Edinburgh)

Suspending motile Escherichia coli in a liquid display 'negative viscosity increment' (NVI) at low shear rate, i.e. adding such bacteria lowers the shear viscosity of the system [1]. At higher concentrations, a regime of near zero viscosity can be reached. Recently, quantitative prediction of this phenomenon has been presented based on an active gel theory (AGT) [2], which also predicts a dependence of the viscosity with the square of the system size. Here, we investigate the system-size dependence of the rheological response of an E.coli suspension as a function of shear rate and concentrations using a low-shear Couette rheometer. Additionally, we image the suspensions in a cone-plate rheo-imaging setup allowing direct visualisation of the collective organisation under shear. We found no size-dependence of the viscosity in contradiction with AGT. Additionally, we found the flow becomes banded and viscosity decreases to near zero at a bacterial concentration in the vicinity of the appearance of collective motion in absence of flow.

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AC23 Collective motion of assemblies of active Brownian filaments

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Active matter systems are comprised of agents which either convert internal energy or absorb energy from the environment and transform it into directed motion. Their associated out-of equilibrium character is the origin of a number of fascinating many-body phenomena present on a broad range of scales: from vertebrates down to motile bacteria, intracellular filaments driven by molecular motors, and enzymatic nano-motors. In particular, active systems with internal degrees of freedom like filamentous, polymer-like structures are involved in various biological processes, e.g., cell motility, and exhibit novel conformational [1] and dynamical properties [2]. A prominent feature is an activity-induced symmetry breaking leading to the spontaneous formation of large-scale structures in the form of clusters. The ability to generate either self-sustained or highly dynamical structures constitutes a generic, distinctive feature of active systems. Our goal is to characterize the collective motion and steady-state out-of-equilibrium patterns in systems of assemblies of active Brownian filaments.

We consider a two-dimensional system of self-propelled Brownian filaments composed of ‘point-like’ self-avoiding particles connected by harmonic springs and bending forces. The dynamics of the system is described by a Langevin stochastic equation of motion in the over-damped regime. The orientations of additional active velocities change independently in a diffusive manner. This allows us to disentangle the role played by self-propulsion, volume exclusion interactions, and bonding/bending intramolecular forces. In addition, we perform a systematic computational study of the phase behavior, and the structural and dynamical properties of such systems.

Supporting recent studies [3,4], our findings endorse a suppression of MIPS with increasing polymer length. Similarly to active Brownian particles, active filaments aggregate more with increasing activity. Surprisingly, stiffer filaments give rise to larger self-sustained clusters. In conclusion, the interplay between particle connectivity, activity and volume exclusion gives rise to a wide range of novel collective phenomena, such as specific cluster formation, highly dynamical structures, collective motion, and even swarming.

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AC24 Spontaneous Behaviour in Electrically-activated Colloids

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Swimmers and self-propelled particles are physical models for the collective behaviour and motility of a wide variety of living systems, such as bacteria colonies, bird flocks, and fish schools. Such artificial active materials are amenable to physical models which reveal the microscopic mechanisms underlying the collective behaviour. Here we study colloids in a DC electric field. Our quasi-two-dimensional system of electrically-driven particles exhibits a rich and exotic phase behavior. At low field strengths, electrohydrodynamic flows lead to self-organisation into crystallites with hexagonal order. Upon self-propulsion of the particles due to Quincke rotation, we find an ordered phase of active matter in which the motile crystallites constantly change shape and collide with one another. At higher field strengths, this turns to an active gas. We parameterise a particulate simulation model which reproduces the experimentally observed phases and, at higher field strengths predicts an activity-driven demixing to band-like structures.

AC25 Role of pH in Microswimming

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Role of pH in Modular Micro Swimming

We have systematically investigated modular microswimmers composed of ion exchange resin beads and cargo particles of different species which self-assemble on charged substrates via pH-gradient driven solvent currents [1]. Starting from experimental data on assembly and propulsion in dependence on boundary conditions like component type, size, charge and cell geometry [2, 3] we initially proposed a qualitative minimal model of assembly and modular swimming [4, 5]. In collaboration with theoretical colleagues working on different approaches we have extended this model to describe several key features in quantified detail. Special focus laid on the underlying pumping mechanism [6], the prediction of swimmer linear and rotational motion from data on the self assembly process [7] as well as on cargo number and distribution influences on the swimming performance with and without gravity [8]. A few interesting results are highlighted presented and future prospect is discussed.

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AC26 Anomalous dynamics of active particles in porous media

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On small length scales, Active matter is a model for both artificial self-propelled particles (i.e. Janus particles, active emulsion droplets) and biological microswimmers, such as motile cells and bacteria. The dynamics of dry active matter in homogeneous and low-Reynolds number environments are well described by Active Brownian motion and run and tumble dynamics. However, natural examples of active matter will be in the presence of walls and obstacles, and thus there is a need to study active dynamics in crowded heterogeneous environments.

In this work we use a complementary combination of both simulation and experiment to study the dynamics of active particles in porous materials. The experiments involve Janus particles flowing through the percolating voids of a colloidal gel. Here, the presence of the gel models environments such as cell cytoskeletons and porous rock. The two methods are further combined by importing tracked gel co-ordinates to act as obstacles for simulated active Brownian particles. Comparing the particle tracking results from these experiments with molecular dynamics simulations, we gain insight into the dynamics and collective behaviours of active matter in random porous environments.

AC27 Effect of long-range interactions on reversible to irreversible transition

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Several periodically driven systems undergo a transition from reversible to irreversible behaviour. An example is provided by non-Brownian colloidal suspensions under low-frequency shear: below a critical density, all particles return to the same position at the end of each cycle; they instead show chaotic motion above. Analogous phenomena are observed in glasses and emulsions.

Minimal models are based on the hypothesis that interactions among colloids are purely local. On this basis, the transition between reversible to irreversible behavior is predicted to belong to the conserved directed percolation universality classes. However, in many experimental realisations, long-range interactions are present, either in the form of hydrodynamics or elasticity. In this work, we discuss their effect using direct numerical simulations and analytical analysis of minimal models.

AC28 The role of topological defects on the two-stage melting and elastic behavior of Active Brownian colloids

PALIWAL, Siddharth (Utrecht University); DIJKSTRA, Marjolein (Utrecht University)

The exact nature of the melting behavior in 2D equilibrium systems has remained quite elusive and debatable in the last few decades but due to recent advances in simulation techniques and hardware it became possible to numerically probe larger length and time scales. It was shown quite recently that a system of hard disks shows a continuous solid-hexatic phase transition followed by a first-order hexatic-fluid transition upon lowering the density[1]. On the other hand, research on non-equilibrium systems of driven granular media and self-propelled particles have identified a rich phase behavior in these systems. The low activity and dilute systems resemble a fluid state with a higher effective temperature and diffusion coefficient whereas the denser states at low activities could condense into a liquid, solid or gel-like state depending on the nature of the particle interactions. This non-equilibrium phase separation of repulsive self-propelled Brownian colloids at high activity has been a theme of great interest especially since the past couple of years. The phase separation is driven by the additional self-propulsion of the particles over their thermal motion and has been termed in the literature as Motility Induced Phase Separation (MIPS).

In this study we examine the phase behavior and structure of a system of repulsive active Brownian particles in two dimensions. In particular, we investigate the role of topological defects on the melting behavior of the active crystalline state. We test the applicability of the well-established Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory of melting in two-dimensional equilibrium systems to the active case as well as the behaviour and properties of topological defects. We find that the intermediate hexatic state predicted for two-dimensional systems not only persists but in fact becomes stable over a wide-density regime upon increasing the activity. Our observations indicate that at high activity the melting transition of the solid phase into the hexatic phase is not driven by the unbinding of bound dislocation pairs. Remarkably, the transition proceeds from the crystalline state into a high-density hexatic state devoid of any defects, but exhibiting short-ranged positional order. Subsequently, the dislocation defects proliferate and introduce plasticity in the system while maintaining the hexatic state. In addition, we find a first-order hexatic-to-fluid phase transition upon lowering the density at low and high activity, whereas this transition becomes continuous for intermediate activities [2,3].

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AC29 Realization of an artificial active bath with controlled activity

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We study the dynamics of an optically trapped Brownian particle in an artificially generated active bath. The particle motion is driven by a thermal noise and an exponentially correlated active noise of tunable duration and strength. Our system thus mimics the motion of a passive particle in a real active bath, such as a bath of swimming bacteria. We measure the mean squared displacement of the particle position and its response to an external perturbation as a function of noise amplitude and correlation time. The change in the effective temperature of the particle as a function of bath activity can be explained by our simple theoretical model based on overdamped Langevin equation. We tested the fluctuation-dissipation theorem and measured the steady state heat dissipation rate as a function of bath activity. Our experiment is significant for the study of various thermodynamic processes in active bath.

AC30 Capillary deposition of microorganisms in a microfluidic channel for the study of cells in spatially controlled environments

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Controlled and precise deposition of microorganisms into defined spatial arrangements offers unique and innovative possibilities for the study of microbial physiology and interactions. Full control over the geometrical arrangement is highly desirable due to the crucial importance of distances in microbe-microbe interactions, arising from their dependence on the propagation of chemical signals. Coupling accurate spatial patterning and full control over environmental conditions would provide a powerful and versatile platform for single-cell studies in microbial ecology. To this end, I have developed a microfluidic platform to extend a capillary deposition technique originally designed for colloidal particles, called sCAPA (sequential capillarity-assisted particle assembly), to bacterial systems. This technology exploits the capillary forces resulting from the controlled motion of an evaporating droplet inside a microfluidic channel to capture individual particles or microorganisms in an array of traps microfabricated onto the substrate. Sequential depositions allow the generation of the desired spatial layout of single or multiple microorganisms. We successfully calibrated this new technique on colloidal particles and tested it on bacteria. We have shown that the coupling of single-cell deposition and microfluidics technology allows both geometric patterning and precise control of environmental conditions, and thus opens up a window into the physiology of single microbes and the ecology of microbe-microbe interactions.

AC31 Enhanced rotational diffusion of squirmers in viscoelastic fluids

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Squirmers are generic models for biological microswimmers and synthetic self-propelled particles [1]. Fluid-mediated interactions are essential for their swimming behavior, which can be strongly affected by the fluid viscoelasticity [1,2]. Experiments on self-propelled Janus particles suggest an increase of their rotational diffusion by orders of magnitude in the presence of a viscoelastic fluid compared to a Newtonian one [2]. We perform mesoscale hydrodynamic simulations of a spherical squirmer in a polymer solution to shed light on the mechanism leading to such an enhancement. The fluid is modeled via the multiparticle collision dynamics (MPC) approach [3] and the added polymers are either of phantom nature or self-avoiding. The concentration of monomers on the squirmer surface is controlled by a short-range attractive squirmer-monomer potential. An increasing attraction strength leads to an enhanced monomer adsorption and a substantial decrease of the rotational diffusion coefficient D_0 of a passive colloid. Interestingly, we find a significant increase in the squirmer rotational diffusion coefficient D_R in the presence of the polymers. Here, self-propulsion not least reduces the monomer concentration on the surface, and hence, leads to accelerated rotational motion. Inhomogeneous collisions with monomers during swimming additionally enhance the diffusion coefficient. We find an increase of the ratio D_R/D_0 up to a factor of 15 for both phantom and self-avoiding polymers. However, excluded-volume interactions imply a weaker enhancement and a decreasing ratio D_R/D_0 with increasing monomer concentration, whereas a monotonic increase of D_R/D_0 is observed in the phantom case. To elucidate the elastic effect of self-avoiding polymers on swimmer's rotation, simulations without squirmer-monomer attraction are carried out, in which the rotational diffusion is enhanced twice. In fact, the observed modulation of the rotational motion could be different from the mechanism observed experimentally [2]. However, our simulations suggest that the rotational dynamics of squirmer-type microswimmers can be controlled by polymer concentration and the degree of adsorption.

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AC32 Transport coefficients of dense active Brownian particles

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We calculate transport coefficients of dense systems of active Brownian particles (ABP). Using an integration-through transients (ITT) formalism, we derive generalized Green-Kubo relations that are valid for the non-equilibrium system granting access to macroscopic quantities like to the viscosity, or the average swim velocity. These Green-Kubo relations are evaluated using a recently developed Mode-Coupling theory (MCT) for the slow dynamics of two dimensional spherical ABP [2]. The key quantity of this theory is the dynamical density-density correlator for which the Mori-Zwanzig projection formalism provides an exact equation of motion containing a convolution with a memory-kernel. MCT is a widely used tool to approximate the memory-kernel [1] which we extended to the case of active Brownian hard disks predicting a glass-transition diagram in the three-dimensional parameter space of density, self-propulsion velocity, and rotational diffusivity. Within MCT, we also calculate mean-squared displacements and obtain the long-time diffusion coefficients. It is possible to study different scenarios: a single ABP in a dense sea of passive or active particles or on the other hand a passive particle driven by a crowd of active particles. The mean-squared displacement shows regimes of sub- and superdiffusion caused by the caging of neighbouring particles and activity. Finally the relation between diffusivity and viscosity is discussed in terms of a generalized Stokes-Einstein relation.

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AC33 Dimeric and trimeric colloids driven by Thermophoresis

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Self-propelled phoretic colloids have recently emerged as a promising avenue for the design of artificial microswimmers. By studying the hydrodynamics of a single swimmer, we can predict the behaviour of large ensembles of colloids. A hydrodynamic fluctuating mesoscale simulation approach is here employed [1]. We present the hydrodynamic velocity fields of various swimmers with different structural shapes. Dimers, rod-like trimers, and v-like trimer are investigated for swimmers with monomers of equal or different sizes in quasi-two and three dimensional systems. The competition between attractive or repulsive hydrodynamic and phoretic interactions varies as a function of the oligomer geometry and phoretic affinity (philic or phobic), which eventually results in a rich phenomenology such as clustering, swarming, or rotational motions [2].

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AC34 Ratchet-induced variations in bulk states of an active ideal gas

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Swimming bacteria and self-propelled colloids are examples of active systems, that constantly convert energy into motion. From a theoretical point of view, these systems are interesting because they are inherently out of thermodynamic equilibrium, and by studying them we hope to learn something about non-equilibrium steady states in general. The game is to look for a system that is as simple as possible, yet displays fundamental features of non-equilibrium states. In this contribution, this system comes in the form of non-interacting active Brownian particles: the active ideal gas. In many cases, an active ideal gas simply behaves as a passive ideal gas at an effective temperature. However, when the particles are placed in a setting with an asymmetric potential barrier, one finds that the potential barrier influences the particle density at arbitrarily large distances – an effect unheard of in equilibrium systems. On this poster [1], we illustrate this effect, and seek to understand it in the simplest setting possible.

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AC35 Active particles at crowded liquid interfaces

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Self-propelling particles have been studied thoroughly in bulk for both diluted and crowded environments [1,2]. Interestingly, particle interactions and their motion are profoundly different at liquid interfaces [3,4,5], especially in the presence of passive obstacles [6]. In this work, we aim to study the behaviour of larger active particles trapped at liquid-liquid interfaces in presence of smaller and passive particles with different packing densities and 2D ordering. The latter is typically characterized by a hexagonal symmetry that allows the active particle to self-propel through the lattice. Remarkably, the passive particles change significantly the interaction landscape of the active analogues, influencing its pathway. By varying the area density of the passive 2D crystal, we can tune both the lattice ordering and the mean distance among the obstacles. We quantitatively analyze how these different environments together with the interaction with the passive particles effect the swimming behaviour of the self-propelling particle.

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AC36 The Effects of Complex Rheology on the Swimming Velocities of a Flagellated Alga

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The motility and the swimming behaviour of microorganisms is greatly influenced by the interactions with the medium in which they live. An understanding of their swimming dynamics in complex media is key for the enhancement of applications such as artificial swimming, micro-robotics and targeted drug delivery. In this work, we examine the effect of rheological characteristics, such as viscosity, viscoelasticity and shear thinning, of the medium on the swimming dynamics of a eukaryotic bi-flagellated puller alga, Dunaliella salina. We make use of dilute algae suspensions, in which alga-alga interactions are not important. To visualise the algae swimming behaviour, we employ microfluidic chambers of rectangular cross-section and rely on microscopy and image analysis to quantify the swimming kinematics. We observe analogous algae swimming velocities and beating frequencies in Newtonian (Ficoll PM400), viscoelastic (Polyacrylamide) and shear thinning (Xanthan Gum) solutions across a substantial range of fluid viscosities. In all cases, swimming velocities decrease as the viscosity is increased up to a point where velocities plateau, exhibiting an approximately constant velocity for high viscosity solutions. These results show a significant divergence to many other swimmers reported in literature. Observations in the shear thinning fluid allows us to further understand the shear responses experienced by this particular swimmer and approximate the characteristic shear rate of the swimmer. Further, we examine the algae behaviour in a second Newtonian fluid (Glycerol). In this case the behaviour is significantly altered, with a more pronounced decrease in swimming velocities as the viscosity is increased and a defined point of non-motility, which was not observed in other cases. We attribute this to cell interactions with the glycerol, changing the make-up of the cell and effecting swimming efficiencies.

AC37 Nucleation and growth in a scalar momentum-conserving active matter

SINGH, Rajesh (University of Cambridge); CATES, M. E.

Active matter systems are driven out-of-equilibrium due to injection of energy at the microscopic scale. We consider a scalar concentration field to describe a continuum theory of active colloidal suspensions, which account for the exchange of locally conserved momentum between the colloids and the solvent. We study the role of active hydrodynamic interactions in determining nucleation and growth in such a field theory and find novel dynamic phases.

AC38 Colloidal transport in heterogeneous landscapes of micro-swimmer activity

Stephen Williams (University of Warwick); Marco Polin (Warwick), Raphal Jeanneret (IMEDEA), Idan Tuval (IMEDEA)

Chlamydomonas reinhardtii, a unicellular biflagellate alga, is widely regarded as a model organism for a broad range of biological and physical studies, from plant photosynthesize to flagellar synchronization, motility (e.g. bioconvection, phototaxis) or active matter. Recently, hydrodynamic entrainment was shown to dominate the effective diffusion of micro-particles embedded in homogeneous suspensions of the algae [1]. Microscopically, the colloids exhibit a dynamics akin to a jump-diffusion process, with successive entrainment events (jumps) interspersed with normal diffusion (slightly enhanced by the far-field flows of the swimmers). In this work we now explore experimentally the effect of *spatially heterogeneous* algal suspensions on the dynamics of weakly Brownian particles by confining the system within quasi-2D microfluidic chambers. In such geometries, the interaction of the swimmers with the confining walls, the interaction of the swimmers with the confining walls [2,3] create a heterogeneous and anisotropic background of diffusion for the colloids. This leads to spontaneous active-passive segregation where the colloids accumulate at the boundaries. This effect can be tuned by fixing the surface-to-volume ratio of the confining channels and can be harnessed to spontaneously demix the active-passive suspension. We rationalize our observations by resolving spatially and temporally the colloidal kicks statistics. Although relatively basic, this experimental system exhibits highly non-trivial out-of-equilibrium dynamics which opens the way to a better understanding and control of passive matter transport by active entities, with potential important applications to e.g. intracellular transport, targeted drug and biomarker delivery or the autonomous depollution of soils.

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AC39 Active Colloidal Circlers

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Active colloids propel themselves through solution by consuming a chemical or physical fuel. While the vast majority of research focusses on active colloids with straightforward motion, we show here that a rotational motion can also be induced using asymmetric Janus colloids created by coating the colloidal monolayer under a glancing angle instead. These active colloidal circlers swim in circles in alternating electric fields due to induced-charge electrophoresis, resulting in chiral swimmers as they are not able to change their direction of rotation. We show that their swimming behavior can be tuned by varying the glancing angle as well as the voltage and the frequency of the applied alternating electric field. In addition, the latter two variables also change their interaction potential from hard spheres into dipolar spheres. The combination of a tunable interaction potential and a rotational motion results in a large variety of dynamically self-assembled structures.

AC40 Active Coacervate Droplets

TESTA Andrea (ETH Zürich, Materials Department, Laboratory of Soft and Living Materials)

Living systems exploit the energy content stored in a chemical fuel (like ATP, glucose, etc.) to carry out useful actions such as performing mechanical work [1]. Taking inspiration from Nature, a broad aim of soft matter science is to design active materials that consume energy to perform functions that are impossible in or near equilibrium [2]. Active coacervate droplets are an attractive option for the formation and study of active materials. Early reported phenomena have included motion, predatory behaviour and light driven catalysis [3-5]. Here we describe a novel system of active coacervate droplets in which metal nanoparticles are partitioned within the complex phase, catalysing the decomposition of a chemical fuel. In particular, we devised a unique method for the synthesis of the nanoparticles such that they are easily functionalized and localized into the coacervate droplets, leading to consumption of fuel that is confined in space. The absence of any membrane between the droplet phase and the environment makes the diffusion of fuel, waste and heat in and out the droplets very fast and efficient, yielding to a sustained activity regime, while the excellent localization of the reaction allows to reach high level of activity density within the droplets. These characteristics make our system an ideal framework for the study of active materials: we will present preliminary results on fuel consumption and mechanical properties.

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AC41 Propulsion of catalytic Janus spheres in viscosified solutions

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The influence of the swimming medium on propulsion at low Reynolds number has been observed for a large number of swimming microorganisms. Beyond the biological realm, studies on low-Re motion of artificial swimmers have also been carried out. For example, the use of Janus particles to make active motors has received much attention. Many applications of such motors involve moving objects through complex environments that are mixtures of components. The flow properties of these mixtures could be Newtonian or non-Newtonian. In other applications, additives may be introduced as a way of controlling the motion of motors. The first step in understanding how the fluid mixtures alter their motion is to examine propulsion in fluids where additives change the shear viscosity while the fluid remains Newtonian. We show how solution viscosity affects Janus motor propulsion keeping all other factors (motor size, fuel concentration, temperature, etc.) constant. The velocity is shown to decay approximately inversely with viscosity. Further, the type of viscosifier used affects the interaction between fuel molecules and motor, which affects propulsion. This is part of the overall goal of understanding how solution properties impact propulsion independent of a particular application. When qualifying the propulsion in crowded environments, it is important to understand how to accurately quantify the response. We have used computer simulations to quantify the errors associated with particle tracking when extracting the propulsion of Janus motors.

AC42 Interparticle torques suppress motility-induced phase separation for rod-like particles

van Damme, Robin (Utrecht University); Rodenburg, Jeroen (Utrecht University); van Roij, Ren (Utrecht University); Dijkstra, Marjolein (Utrecht University)

As an exemplary active matter phenomenon, motility-induced phase separation (MIPS) has received significant attention over the last few years. MIPS emerges in model systems of strongly self-propelled disks and spheres, regardless of whether their self-propulsion mechanism is run-and-tumble or active Brownian, and regardless of the specifics of the interactions between the particles. Given this fact, it is tempting to think that MIPS emerges in any system with strong self-propulsion. However, that is not the case. The robustness of MIPS in these model systems is because they are isotropic: they have no torques acting between particles. Here, we demonstrate the surprisingly strong dependence of MIPS on interparticle torques. For self-propelled repulsive rod-like particles, MIPS is suppressed entirely once the rod aspect ratio exceeds approximately 2. We propose an intuitive (though still somewhat handwavy) explanation based on the duration of particle collisions, and argue that this can explain both the suppression of MIPS found here for rod-like particles and the enhancement of MIPS found for particles with Vicsek interactions.

AC43 Filamentous Active Matter: Band Formation, Bending, Buckling, and Defects

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Motor proteins drive the persistent motion of cytoskeletal filaments in vivo as well as in vitro. We perform component-based Brownian dynamics simulations of polar semiflexible filaments and molecular motors. This allows for linking the microscopic interactions and the filament activity to self-organisation and dynamics from the fundamental two-filament level all the way up to the of mesoscopic domain level. Dynamic filament crosslinking and sliding, and excluded- volume interactions promote formation of motor-bound bundles at small filament densities, and of active polar nematics at high densities. An Euler buckling-type instability sets the size of the polar domains and the density of topological defects. We predict a universal scaling of the active diffusion coefficient and the domain size with the active force, and its dependence on parameters like motor concentration, filament concentration and persistence length.

AC44 Active Brownian Particles at High Densities

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Active Brownian Particles (ABP) undergo passive Brownian motion combined with directed motion along a randomly reorienting body axis. They comprise arguably one of the simplest models to study the effect of ‘active’ driving forces in classical statistical physics. Intriguing non-equilibrium phenomena are observed in ABP systems, among them a motility-induced phase separation (MIPS) and kinetic arrest, i.e., the transition from the homogeneous fluid to an ‘active’ glass. We discuss the high-density dynamics of ABP with the help of Brownian dynamics simulations and of a mode-coupling theory for the active glass transition. The theory predicts kinetic arrest that depends non-trivially on the interplay between the persistence length of the active motion and the caging length set by excluded-volume interactions. Combined with the integration-through transients (ITT) mechanism that allows to systematically derive Green-Kubo like expressions for non-equilibrium transport coefficients, a state diagram comprising both kinetically arrested and phase-separated states. Simulations reveal that the kinetic-arrest transition predicted by the theory separates qualitatively different regimes for the long-time dynamics with regard to the dependence of the paramters controlling the particles’ activity. We link this to a discussion in how far kinetic parameters of the motion (such as short-time diffusivities) enter the long-time fate (fluid or glassy) of high-density states.

AC45 Active Brownian particles: Local pressure in nonequilibrium systems

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Motile active systems develop an intrinsic swim stress through their locomotion, which influences their dynamics and collective behavior [1,2,3]. Such stresses are particularly interesting, since there is no equilibrium counterpart and, thus, no thermodynamic description exists. The stress of a fluid on a confining wall is given by its mechanical wall forces, independent of the passive or active nature of the fluid [3]. In systems at thermal equilibrium, an equation of state exists and local stress can be defined via Clausius' virial theorem or thermodynamically by the Helmholtz free energy. However, for non-equilibrium active systems, a comparable local description is missing, which has hampered the characterization of inhomogeneous active systems.

We derive an expression for the active stress in a local volume inside of a confined, wall-bound system of spherical active Brownian particles (ABPs) [4]. On the one hand, we find a new virial expression for the local active stress, and, on the other hand, we identify an original active-momentum contribution due to particle flux across a virtual plane. The local stress is quantified in computer simulations of non-interacting ABPs and ABPs interacting by a short-ranged repulsive Lennard-Jones potential. We demonstrate that the stress on the wall and the local bulk stress are identical, which confirms the existence of a pressure equation of state for spherical ABP systems. Most importantly, our calculations demonstrate that active pressure is not a boundary effect, but is caused by momentum transport due to activity. Moreover, it opens up the possibility to calculate stresses locally, even in inhomogeneous systems, which we confirm by calculating the local stress in a phase separated system of ABPs.

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AC46 What changes the collective behaviour of a group of zebrafish

YANG, Yushi (University of Bristol); ROYALL, Paddy; Russo, John

A large group of living animals such as birds, midges and fish can be think of being active matter since they are made up of self-driven individuals that take energy from the environment to produce movement. [1] In the nature, these animals exhibit ordered and disordered collective behaviours, such as flocking and swarming. [2, 3] We studied the collective behaviour of a large group of zebrafish (group size ranging from 5 individuals to 100 individuals) in the laboratory. The fish were allowed to swim in three dimensional space and a quasi two dimensional space (shallow fish tank). The order of their movement was characterised by the translational, rotational and dilatational order parameter, which were measured from the trajectories of the fish. The orientational correlation of fish were also measured experimentally. The fish school exhibits different collective moving order and correlation lengths depending on the group size, environmental brightness and the dimension of the space in which the fish swim.

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AC47 Non-equilibrium, driven self-assemblies in an oil-in-oil emulsion

YETHIRAJ, Anand (Memorial University of Newfoundland); Somayeh Khajehpour Tadavani

Non-equilibrium self-assemblies in soft materials emerge in the presence of a driving force and viscous dissipation. In a series of experiments [1-6], we have explored in depth a simple oil-in-oil emulsion where an external electric field can yield a rich variety of ""tunability"": i.e., frequency-controlled hydrodynamics, that yields different dynamical regimes and structures:

- from drop breakup to drop coalescence
- from crystals to disordered structures
- from 2D motions to convection to turbulence.

All are controlled by the super-diffusive motions of the underlying fluid (measured by tracer-particle flows).

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AC48 Systems with broken third Newton's law: Dissipative phase transitions and particle-resolved studies with complex plasmas

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KRYUCHKOV, Nikita P. (Bauman Moscow State Technical University);
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The reciprocity of effective interparticle forces can be violated in various open systems, from active soft matter (colloidal suspensions and complex plasmas) to social systems and networks. In this talk we consider the generic dynamics of such systems and demonstrate a criterion under which a nonreciprocal system can be strictly reduced to a pseudo-Hamiltonian system with detailed dynamic equilibrium. When this criterion is not satisfied, the steady state is determined by the interplay between dissipation and energy source due to the nonreciprocity of interactions. The results indicate the realization of bistability and dissipative spinodal decomposition in a broad class of open systems with nonreciprocal effective interactions and, in particular, in complex (dusty) plasmas [1]. Using two-dimensional (2D) complex plasmas as an experimental model system, we carried out particle-resolved studies of flame propagation in classical 2D solids and thermoacoustic instability in fluids [2, 3]. Combining experiments, theory, and molecular dynamics simulations, we demonstrate that the due to nonreciprocal interactions, operating in the system, 2D complex plasmas reveals all essential features of combustion, such as an activated heat release, two-zone structure of the self-similar temperature profile ('flame front'), as well as thermal expansion of the medium and temperature saturation behind the front. Moreover, 2D complex plasma fluids demonstrate thermal activation behavior that can result in thermoacoustic instability, recently reported in [3]. The results are of relevance for various fields ranging from combustion and thermochemistry, to chemical physics and synthesis of materials, and indicate a deep physical analogy between collective fluctuation dynamics in reactive media and in systems with nonreciprocal effective interactions exposing an activation behavior. Project is supported by RSF Grant no. 17-19-01691.

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AC49 Design and synthesis of catalytically active CoFe2O4@Pt nanostructures

MARTINEZ, Yeimy (Unversity of Cologne); QUILITZSCH, Lars (University of Cologne); EFFERTZ, Marc (University of Cologne); SCHMIDT, Annette (University of Cologne)

The controlled motion of active micro- and nanostructures in aqueous solutions is of interest for both fundamental research and emerging biomedical applications. Nature has inspired numerous designs founded on the swimming patterns and self-propulsion of biological swimmers. Mimicking these features might thus enable the design of active structures that propel themselves by taking up energy from their surroundings and transforming it into directed motion.[1] Within this approach, considerable research is focused on the design of catalytically active and geometrically asymmetric Janus particles.[2] In general, the advantage of these systems lies in the possibility to catalyze chemical reactions at only one side of a particle, thereby producing a driving force that impulses it forward resulting in a self-propelled object. Herein, we present novel heterofunctional CoFe2O4@Pt nanostructures activated through a novel chemical fuel system based on the catalytic reduction of borohydrides. The nanostructures are prepared via a seed-mediated growth process, which entails a stable interface linkage between the CoFe2O4 and Pt domains.[3] The propulsion is generated by a concentration gradient considering fuel and reaction products in the vicinity of the catalytic nanoobject, and by railing their direction using a homogeneous magnetic field. This investigation includes the systematic synthetic approach implemented to prepare nanostructures in a size range smaller than 50 nm, the development of a new fuel system and the real-time tracking of the motion using dark-field light scattering microscopy.

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AR1 The emergence of cooperativity accompanying vitrification: Insights from density fluctuation dynamics

Akira Furukawa (University of Tokyo)

We discuss the emergence and growth of the cooperativity accompanying vitrification based on the density fluctuation dynamics for fragile glass-forming liquids. (i) The relaxation of density fluctuations proceeds by the particle (density) exchange process, and is diffusive; that is, the allowable kinetic paths are strongly restricted by the local conservation law. (ii) In normal liquid states, this exchange process is less cooperative, and the diffusion coefficient of density fluctuations D_c is given as $D_c \sim \lambda^2/\tau_\alpha$, where λ is the particle size and τ_α is the structural relaxation time. On the other hand, in supercooled states the restriction on the kinetic path is more severe with increasing the degree of supercooling, which makes the exchange process more cooperative, resulting in $D_c \sim \xi_{\mathrm{d}}^2/\tau_\alpha$ with ξ_{d} being the cooperative length scale. (iii) The molecular dynamics simulation results show that the self-diffusion coefficient of the tagged particle, D_s, almost coincides with D_c, suggesting that the collective density diffusion and the particle diffusion closely share the same mechanism: in normal states D_s determines D_c, but vice versa in supercooled states. This immediately leads to the idea that the breakdown of the Stokes-Einstein relation is not the anomaly in the single-particle dynamics but reflects the increase in the cooperativity in the density diffusion at the length scale of ξ_{d}.

AR2 Dynamical arrest in binary colloidal system with static and dynamic cages.

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We have simulated a binary spherical colloidal particle in which one fraction of particle form irreversible bonds while the other fraction interacts only via hard core repulsion. We will show that the aggregating species have a fractal dimension of 2 in the flocculation regime while in the percolation regime it has a fractal dimension of 2.5. When the kinetics of the aggregating species was arrested we restarted the system and the dynamics of the hard sphere within the cages of the percolated network was investigated for 2 cases. In one case the percolated cluster was freezed or cages were static and diffusion of the hard sphere was looked which showed similar behavior as the dynamics of the tracer particle in crowed environment. In the second case the dynamics of the particles within the bonds was allowed for the percolating network or the cages were dynamic and diffusion of the hard sphere fraction was studied. The hard spheres showed anomalous diffusion in both the cases. In the static cage case below a certain fraction of hard sphere the dynamics were arrested, where the particles where stuck inside the cages and never escaped from the cages. For the case of dynamic cages we will show that for small fraction of the hard sphere the intermediate scattering function shows a double relaxation similar to colloidal glass transition for volume fraction above 0.3 and for higher fraction hard spheres we were only observing a stretched exponential behavior. Also in the dynamic cages we will show that most of the hard sphere particles are only temporarily stuck inside the cages and will diffuse in and out of the cages.

AR3 Reinforcing Soft Gels

DAMERAU, Brian (Georgetown University); BANTWANA, Minaspi (Georgetown University); DEL GADO, Emanuela (Georgetown University); BISCHOFBERGER, Irmgard (Massachusetts Institute of Technology); DIVOUX, Thibaut (Massachusetts Institute of Technology)

We investigate the rheology and the microscopic dynamics of nano-composite gels. Introducing micron-sized fillers (particles, fibers, etc.) has proven to be a major av-enue for the modification/enhancement of the mechanical response of composite mate-rials. Nano-composites that use soft gel matrices and nanoscale fillers are especially in-teresting, since they withstand large deformations. We have designed a computa-tional approach to complement on-going experiments, which explore the dynamics of nano-composite gels for a wide range of volume fractions and filler sizes. We analyze the roles of the filler-matrix interactions and the microscopic dynamics on the rheology of the composite material.

AR4 The Impact of Hydrodynamics on Colloidal Gelation under Gravity

DE GRAAF, Joost (Utrecht University); ZHOU, Xuemao (University of Edinburgh); HERMES, Michiel (Utrecht University); POON, Wilson (University of Edinburgh)

The stability of gels formed by colloidal particles with short-ranged interactions is of importance to a wide range of industrial applications. These systems are intrinsically out of thermodynamic equilibrium and therefore have a finite shelf life, determined by the onset of (rapid) sedimentation under the influence of gravity. Yet, many of the processes underlying this gel collapse remain poorly understood.

Recent experiments show that fluid flow plays a major role in the loss of structural integrity of the gel [1,2]. Concurrent improvements in computational performance have made it possible to numerically study the influence of hydrodynamic effects on gel formation [3,4] and gel collapse [5]. Using the lattice-Boltzmann technique, we have demonstrated that hydrodynamic interactions influence the dynamics of gelation, but not the gel structure [6].

Here, we go beyond our previous results [6] and numerically study the formation of colloidal gels under the influence of gravity and in the presence of hydrodynamic effects. We report a dynamic stability criterion for gel formation: below a critical volume fraction fluid back flow interferes with gel formation and the colloids rapidly sediment, above the system gels sufficiently quickly for mechanical strength in the gel network to resist gravity. Remarkably, the effect of the fluid is negligible in the latter regime. The critical volume fraction is a function of the gravitational Pclet number and we relate our dynamic stability line to our experimental observations of gelation.

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AR5 Thermoresponsive gelation of pNIPAM microgels in the presence of non-ionic surfactant

Fussell, Sian (University of Bristol); BAYLISS, Katie (University of Bristol); LI, Wei (Capital Normal University); FAERS, Malcolm (Bayer AG); ROYALL, C. Patrick (University of Bristol); van Duijneveldt, Jeroen S. (University of Bristol)

Understanding gelation of colloids is a long-standing challenge in soft matter. A variety of mechanisms have been postulated [1], and often, the mechanism of spinodal decomposition is found in mixtures of colloids and other species, including polymers, arrested due to locally rigid arrangements of particles [2]. However, other mechanisms are also possible, for example gelation due to polymer bridging [3]. Here we investigate the temperature dependent gelation of mixtures of pNIPAM microgels and a non-ionic polymeric surfactant.

pNIPAM is a temperature responsive polymer that, when synthesised to form cross-linked microgels, has a volume phase transition temperature around 32 °C, where the particles deswell with increasing temperature and expel water from their interior [4]. Due to the temperature response being close to physiological conditions, pNIPAM research often investigates its potential for biomedical applications [5].

It was recently discovered that at temperatures in excess of the volume phase transition temperature, mixtures of pNIPAM and polymeric surfactant undergo a transition from transparent liquid to solid gel, this transition is fully reversible [6]. The gelation is also accompanied by a change from transparent liquid to opaque white solid, the gels that result are initially space spanning but collapse over a time scale much greater than the collapse of the pNIPAM microgels.

Our investigations reveal that the gelation results from the association of the two species in solution, rather than that of the common gelation regime due to depletion, where non-adsorbing polymer causes colloidal aggregation. This association is highlighted by an increase in the hydrodynamic radius of the pNIPAM particles in the presence of the surfactants above the volume phase transition temperature. Confocal microscopy of fluorescently labelled polymers showed that both species are present in the gel network.

Here we use synthetic techniques to alter the architecture of the pNIPAM particles, in order to gain greater insight into the gelation mechanism. In particular, we investigate that the effect cross-link distribution has on the behaviour of the pNIPAM particles. It was found that in particles with a uniform cross-link distribution the gelation mechanism is hindered, and the pNIPAM particles remain stable individual particles in solution. This adds further weight to the hypothesis that the temperature responsive association of the species is responsible for the gelation. This result also highlights that the diffuse corona of the microgels plays a role in the association that drives gelation takes place. The structures that result from this gelation have thin, elongated branches compared to more compact structures commonly found in depletion gels, indicating possible tissue engineering applications.

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AR6 Critical dynamics of active microrheology in a colloidal glass

GRUBER, Markus (University of Konstanz); ABADE, Gustavo (University of Konstanz); FUCHS, Matthias (University of Konstanz); PUERTAS, Antonio (Universidad de Almera); SCHEFFOLD, Frank (University of Fribourg); SENBIL, Nesrin (University of Fribourg); ZHANG, Chi (University of Fribourg)

To access the local dynamics in a colloidal glass, we study the motion of a probe particle of the same size. Driving the particle by an external force allows us to study nonlinear phenomena like the depinning of the particle. While being non-ergodically caged by its neighbors for small forces, the probe will eventually push them away and move through the system for large forces. The critical force separates these two regimes with a very different phenomenology, which is investigated using mode coupling theory (MCT), Langevin dynamics simulations and experiments with a polystyrene particle in an emulsion glass [1].

Based on the MCT analysis [2], we present several methods to identify the critical force in non-ideal systems, which are tested in the simulations and experiments. They yield consistent results. Around the critical force, the mean displacement is neither constant, as expected for a solid, nor proportional to the time, as expected for a fluid, but grows like a fractional power. This can be understood by analyzing not only the first moment, but the full probability distribution of the particle positions, the van Hove function. It shows exponential tails below the depinning transition, which transform into a transient bimodal structure above the depinning transition. This does not only affect the mean displacement, but also causes a superlinear increase of the reduced MSD. Finally, a strong correlation between the critical force and the strength of the local cages could allow predictions of the macroscopic yield stress.

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AR7 Non-equilibrium states of protein solutions: phase separation and dynamical arrest

HANSEN, Jan (Heinrich-Heine-University Duesseldorf); MOLL, Carolyn (Heinrich-Heine-University Duesseldorf); PLATTEN, Florian (Heinrich-Heine-University Duesseldorf); EGELHAAF, Stefan U. (Heinrich-Heine-University Duesseldorf)

Soft materials can form amorphous solids, e.g. gels and glasses, which are relevant for such diverse fields as food engineering, pharmaceutical industry and materials science. To analyze the non-equilibrium states of colloidal particles interacting via short-ranged attractions, we use a monodisperse suspension of nearly spherical particles, namely globular proteins (lysozyme). The metastable gas-liquid binodal as well as the attractive glass line have been determined and the second virial coefficient B2 has been measured for various solution conditions, i.e. salt concentrations, by optical microscopy, centrifugation experiments and light scattering respectively. If the temperature axis of the binodals is expressed in terms of B2, binodals obtained under various conditions fall onto a master curve, as suggested by the law of corresponding states [1]. For colloids with short-ranged attractions, gelation has previously been related to gas-liquid phase separation and a universal state diagram has been proposed if scaled by B2. However, this is in contrast to our findings. Arrest lines for different salt concentrations overlap within experimental errors, whereas they do not overlap if the temperature axis is replaced by B2. This indicates that the binodals are not sensitive to the details of the potential, but can be described by one integral parameter, i.e. B2. In contrast, the arrest line appears to be governed by the potentials attractive part.

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AR8 Glass to liquid transition in model matrix-free polymer grafted nanoparticle systems

JHALARIA, Mayank (Columbia University in the City of New York); FYTAS, George (Max Planck Institute for Polymer Research); BENICEWICZ, Brian (University of South Carolina); KUMAR, Sanat (Columbia University in the City of New York)

Recent work has shown that materials comprised only of nanoparticles densely grafted with polymer chains (GNPs) possess unusual properties. Their gas permeability shows nonmonotonic behavior with increasing polymer length, with peak permeabilities of 8-20 times relative to the neat polymer, depending on the probe penetrant. This behavior has been observed for a variety of graft polymers, core sizes and grafting densities thus indicating a potentially universal behavior for such composites. Using a combination of X-Ray Photon Correlation Spectroscopy, Brillouin Light Scattering and Inelastic X-Ray Scattering we can probe the collective dynamics of these systems and show that these systems undergo a transition from a colloidal glass to a liquid with increasing polymer chain length at constant grafting density. Infact, this transition is reflected in the static structure of the system where a hard sphere order parameter based on the first peak of the structure factor shows a similar melting transition as seen from the dynamics studies as well as suppression of long range density fluctuations for shorter chains . This transition manifests itself in a host of anomalies in the fast relaxations (ps ? ns) of the tethered polymer chain due to distortions of the polymer corona in the jammed colloidal system. Different ways of accessing such jammed colloidal systems are also discussed, using a combination these model colloids and small fractions of short polymer chains.

AR9 Quantifying the mechanical disorder of solids

KAPTEIJNS, Geert (University of Amsterdam); LERNER, Edan (University of Amsterdam); BOUCHBINDER, Eran (Weizmann Institute of Science)

Systems of particles that resist persistent shear deformations are conventionally considered to be solids. With the exception of perfect crystalline solids, most solids found in the physical world feature some degree of disorder, whether intrinsic, or induced by the presence of defects. Solid systems span a very large breadth of characteristic length and energy scales; it is therefore important to be able to quantify on an equal footing the degree of mechanical disorder that these system may possess. In my talk I will introduce two theoretical frameworks to quantify the mechanical disorder of solids, both based on long-wavelength elasticity: one valid for large but finite systems, the other valid in the continuum limit. I will show that the two measures of mechanical disorder depend in the same way on different knobs of disorder, establishing their universal applicability, and establishing a relation between finite-size and continuum effects of disorder.

AR10 Controlling the Morphology Evolution of a Particle-Stabilized Multi-Component System

Li, Tao (Institute of Physics, Chinese Academy of Sciences)

Arrested composites can be created via the stabilization of convoluted fluid-fluid interfaces, which applies to multiple immiscible liquid systems containing dispersed colloidal particles. Such systems can form various morphologies, including the conventional Pickering emulsions, multiple emulsions, Janus droplets and non-spherical droplets. Moreover, the jamming of interfacial particles provides a promising route to create even more elaborate arrested states. For instance, the bijels (bicontinuous interfacially jammed emulsion gels). All these structures exhibit novel properties and can lead to numerous applications in drug delivery, food, energy conversion and functional materials.

Part I of this talk will focus on the viscosity effect on the formed structures in a binary liquid system, which reveals the formation mechanism of bijels created by direct mixing, and fills an important gap between the phase behaviors in low molecular weight liquids and that in bulk polymers. When mixing three immiscible liquids, the morphology development becomes more complex. In Part II, I will introduce both the formation mechanism and the stability mechanism of Janus emulsions, which can be a combined effect of multiphase immiscibility, interfacial tensions and surface stabilization.

AR11 Particle concentration effect on the T1 events' distribution in foams

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Fluid foams consist of a collection of gas bubbles dispersed in a continuous phase which tends to minimize its surface energy under the volume constraint. They exhibit a solidlike behaviour given that they can support small stress, but they can also flow under sufficiently large shear like a fluid does. As the applied shear increases, the bubbles are distorted and elastic energy is stored given the increasing of the total interfacial area. Above a critical applied stress, a pair of adjacent bubbles can be squeezed apart by another pair, giving rise to dissipation of energy. These elementary plastic events or topological rearrangements are known as T1 events.

We use a Hele-Shaw cell of radial geometry, made of two horizontal acrylic plates separated by a gap thin enough that the bubbles are confined as a monolayer. The inlet is located at its center forcing that the foam flows from the center to the outer edge. We observe a radial distribution of T1 events, which is proportional to the velocity squared. On the contrary to previous experiments [1], the preferred direction of the T1 events is perpendicular to the flow direction. It is well known that adding particles to the liquid has a stabilizing effect on the thin films [2,3]. Here we explore the particle concentration effect on the spatial distribution of T1 events.

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AR12 Exploring rotational dynamics in glassy patchy particles systems

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When we cool down or compress a liquid sufficiently rapidly, dynamics slow down as particles become trapped in cages formed by their neighbors. In systems with directional interactions, such as patchy particles, these cages limit both the translations and rotations of each particle. Hence, using patchy particles as building blocks for supercooled liquids allows us to explore the complex interplay between rotational dynamics and dynamical arrest. Moreover, directional interactions provide a route for controlling the local structure and dynamics of the liquid, as they can reinforce the formation of the long lived icosahedral clusters, which dramatically slow down the relaxation of the system [1]. Here, we explore the effect of directional interactions on the dynamics and local structure of dense patchy fluids. We use extensive molecular dynamics simulations to investigate patchy particles with two distinct patch geometries: one which favours icosahedral local structures, and one which does not enhance any particular local structure. For the first case, we find an optimal angle that maximizes the formation of icosahedral clusters, resulting in extremely slow dynamics. Additionally, we show from our simulations that the rotational relaxation is decoupled from translational relaxation in nearly all cases. We conclude that while translational dynamics are controlled by collective effects, the rotational relaxation is purely dependent on the local structure.

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AR13 Parametric Modelling of Phase Transitions

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Nowadays, the theory of supercooled liquids and glasses, proteins and molten polymers, and other complex nanomaterials is under intensive developing by means of computer simulations and macroscopic parametric modelling. We examine the generalized parametric model based on the Landau-type kinetic potential as a function of fourth degrees involving four control and two order parameters with application to the first order phase transition. One shall adopt the most convenient general form allowing one to study phase transitions in the presence of an intermediate metastable state before settling to the final state, because both the order and control parameters are significantly different for distinct physical systems, e.g. anomalous generation and extinction phenomenon of crystal nuclei at very low temperatures in non-equilibrium supercooled liquids containing hydroxyl group, namely o-benzylphenol, salol, and 2,2'-dihydroxybenzophenone [1-3]. Comprehensive presentation of these issues is done in [4-8]. Real solutions representation of the cubic equation with real coefficients is given in parametric form, which is more convenient for the solutions analysis, investigating their dependence on the equation coefficients, i.e. parameters of the thermodynamic systems under investigation, and realizing direct calculations with the use of computers. One can notice that the parametric representations of real solutions for the given cubic equations are significantly more convenient in the implementation of practical calculations than the well-known traditional Cardano's representation, and, in such a way, the given parametric form along with Cardano's formula can be used as analytical expressions for the solutions of the cubic equation with real coefficients. The presented results refer to the complete list of canonical forms and bifurcation diagrams, as well as the sensitivity analyses of the ordinary and bifurcation equilibrium values of the order parameters as a function of control parameters, and the estimation of the phase transition time. This fact may be significant in interpreting the experimental observations in non-equilibrium supercooled liquids. For example, classical nucleation theory, which predicts an extremely slow nucleation rate below the glass transition temperature, cannot explain anomalous nucleation phenomena in supercooled liquids. Moreover, the presence of heterogeneity in the nucleation of protein crystals can be described by a structural order parameter, and model predictions could be tested in the appropriately designed experiments. These results are also relevant, in particular, to selecting storage conditions in order to ensure the physical stability of amorphous drugs, and this motivates a fundamental understanding of crystallization in deeply supercooled liquids and molecular glasses [9].

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AR14 Chain-length dependent rheology and relaxation dynamics in glass-forming oligomers and polymers

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Understanding how a glass is formed on a microscopic level remains an outstanding problem in condensed matter physics; both the approach towards the glassy state and the molecular behaviour within the glass remain to be fully understood. Moreover, how chain connectivity in oligomers and polymers affect the relevant molecular behaviour is not presently clear. The work presented here addresses these questions through a systematic experimental study ranging from small molecules to oligomers and polymers, including molecular systems of different characteristics (flexibility, fragility, etc). The effects of molecular chain-length on the rheology and chain, structural and secondary relaxations are explored using a range of experimental techniques. Results attained from rheology, broadband dielectric spectroscopy and calorimetry will be discussed, outlining their role in determining the material response for molecules of different chain-length and chemistries. The work will be presented in the context of established models and behaviour previously reported in the literature.

AR15 Numerical prediction of colloidal phase separation by direct computation of Navier-Stokes equation

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Numerical prediction of the physical properties of liquid-containing soft materials, such as colloidal gels, which are formed by phase separation, is highly desirable but challenging. However, it is quite challenging primarily because the motions of the components at different hierarchical levels (e.g., large colloids and small solvent molecules) are spatio-temporally coupled in a complicated manner via momentum conservation. Here we critically examine the predictability of numerical simulations for colloidal phase separation as a prototype example of self-organization of soft materials containing a liquid. To this end, we compare the kinetic process of colloidal phase separation between experiments and simulations at the same thermodynamic conditions on the basis of single-particle-level structural information. We perform both three-dimensional time-resolved confocal-microscopy observations and hydrodynamic simulations in which a solvent component is coarse-grained as a continuum. We find that after matching the inter-colloid potential and temperature in the simulations to reproduce the thermodynamic behaviour of the experiment systems, our hydrodynamic simulations almost perfectly reproduce the structural and topological evolution processes of the experiments without any adjustable parameters for both dilute and semi-dilute suspensions. Furthermore, comparison with non-hydrodynamic simulations shows the fundamental importance of many-body hydrodynamic interactions in the structural evolution of colloidal phase separation. The predictive power of our computational approach may significantly contribute to not only the basic understanding of the dynamical behaviour and self-organization of soft, bio, and active matter but also the computer-aided design of colloidal materials.

AR16 Low density Colloidal Coulomb Glasses

Thomas Palberg (Institute of Physics, JGU, Mainz Germany); HEIDT, Sabrina (JGU Mainz), BOTIN, Denis (JGU, Mainz) NIU, Ran, (Cornell)

Colloidal glasses formed from hard spheres, nearly hard spheres, ellipsoids and platelets or their attractive variants, have been studied in great detail. Complementing and constraining theoretical approaches and simulations, the many different types of model systems have significantly advanced our understanding of the glass transition in general. Despite their early prediction, however, no experimental charged sphere glasses have been found at low density, where the competing process of crystallization prevails. We here report the formation of a transient amorphous solid formed from charged polymer spheres suspended in thoroughly deionized water at volume fractions of 0.0002 - 0.01 [1]. From optical experiments, we observe the presence of short-range order and an enhanced shear rigidity as compared to the stable polycrystalline solid of body centred cubic structure. On a density dependent time scale of hours to days, the amorphous solid transforms into this stable structure [2]. We further present preliminary dynamic light scattering data showing the evolution of a second slow relaxation process possibly pointing to a dynamic heterogeneity known from other colloidal glasses and gels [3]. We compare our findings to the predicted phase behaviour of charged sphere suspensions and discuss possible mechanisms for the formation of this peculiar type of colloidal glass.

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AR17 Microstructure and Dynamics of Magnetic Nickel-Silica Janus Particles in a Static Magnetic Field

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Magnetic Janus particles were recently brought into focus because of their potential use in many applications by virtue of their responsiveness to externally applied fields [1,2,3]. For instance Janus particles bearing two distinct physical properties are widely used in tissue engineering [4] or display technology [5]. A change of the material properties is often related to an alternation of its dynamic characteristics which are strongly coupled to a variation of the particle-particle interactions with respect to the externally applied field. Hence, even for relatively simple systems consisting of spherical colloidal Janus particles this leads to a much more complex structural and dynamic behavior owing to the influence of the external field. While microscopy is a powerful tool to investigate such systems the dynamics of smaller entities is much harder to scrutinize. However, modern synchrotrons providing a high coherent photon flux and fast detector electronics allow to access the relevant time scales of such systems [6] in order to study their dynamic behavior on the microscopic length scale. Here we focus on the dynamics of magnetic silica/nickel Janus particles in aqueous solution in a static magnetic field by multi-speckle ultra small-angle X-ray photon correlation spectroscopy. In particular the dynamics of the Janus particles is investigated when the magnetic field is applied perpendicular to the incident beam direction. The intrinsic magnetic dipoles of the Nickel caps lead to complex magnetic interactions between the individual particles. Thus, particles already orient at relatively weak magnetic fields and assemble into chain-like structures with directional binding along the field direction [7]. As a function of magnetic field the measured static small-angle scattering pattern increasingly evolve with an anisotropic structure factor arising from the anisotropic pair correlations induced by the complexity of the magnetic dipole-dipole interactions. Furthermore the experimentally obtained intensity-intensity autocorrelation function changes from an initially single-exponential relaxation behavior to a more complex multi-step relaxation pattern with glass-like features. Two distinct relaxation times could be identified. Where at intermediate times a plateau develops as a function of magnetic field, indicating a transient trapping of particles in the aligned chain-like aggregates. Hence the short time behavior on a millisecond time-scale is interpreted as the Brownian ?rattling? inside the chain structure and only at sufficiently long times the particles escape and thus the autocorrelation function fully decays.

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CO1 Competing solidification and fractionation kinetics in hard sphere melts

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Fluid to crystal first order phase transitions of monodisperse hard spheres (HS) upon increasing volume fraction was predicted in the 1950s and later confirmed experimentally on sterically stabilized HS approximants [1]. In experimental hard sphere approximants, size polydispersity is unavoidable. This has significant effects on their phase behavior. Theoretically, above a terminal size polydisperity of about 7%, the formation of coexisting crystal phases is expected, while at lower polydispersity a fluid still coexists with these [2]. We here study a moderately polydisperse (6%) microgel system swollen in a good solvent. Uncharged and excellently buoyancy matched, this colloidal system is less prone to jamming effects than other common HS approximants [3]. We compare its crystallization behavior at two different volume fractions: one directly at the fluid - single solid phase boundary, the other in the fully crystalline regime. For both samples, time resolved static light scattering revealed several series of well indexable narrow Bragg reflections. In the first sample these appear shortly after shear melting and prevail over extended times, before they yield to a more randomly stacked solid with scattering patterns well known from studies using PMMA-based hard sphere approximants. This demonstrates the initial existence of crystals with same fcc structure but different lattice constants and a subsequent stress relaxation via twinning. The second sample initially shows r-hcp scattering patterns, but on long time scales evolves additional indexable series of narrow reflections. Despite the location of the samples in a single crystalline phase region of the phase diagram, we thus observe indications of a significant influence of local solidification kinetics biasing a very narrow particle size distribution in individual crystals. This calls for revisiting the notion of fractionation as such.

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CO2 Revealing hidden structures with unsupervised learning

BOATTINI, Emanuele (Utrecht University); DIJKSTRA, Marjolein (Utrect University), FILION, Laura (Utrecht University)

The study of many structural and dynamic phenomena involving crystalline phases, including nucleation and growth, melting and grain boundary dynamics, relies on our ability to determine whether or not a particle is part of a crystalline cluster or domain. In bulk, crystalline solids can be straightforwardly distinguished from fluids as they exhibit both translational and bond-orientational order. However, on a single-particle level, the distinction between a fluid and a crystal is much less clear: in a small crystalline cluster, as might exist during nucleation, long-range translational or bond-orientational order is not present. Machine learning has been shown to be an extremely promising approach in the study of phase behaviour, both for predicting phase transitions as well as for developing new order parameters. Here, we use unsupervised learning techniques in order to detect distinct particle environments associated to different crystalline and fluid phases.

CO3 Complete density dependence of charged sphere colloid electrophoretic mobilities

BOTIN, DenisJohannes Gutenberg-Universitt Mainz (JGU Mainz); WENZL, Jennifer (JGU Mainz); PALBERG Thomas (JGU Mainz)

Previous reports on the density dependence of the electro-phoretic mobility of charged spheres gave contradicting results. In studies on isolated particles in either aqueous [1] or organic solvent [2], very small mobilities were observed. Starting from very low concentrations, the mobility was found to first increase, but then to saturate with increasing particle number density, n [3, 4, 5]. There, the transition to a concentration independent mobility seems to correlate to the onset of inter-particle ordering, i.e. to conditions of strongly overlapping electric double layers. Moreover, increase and saturation have been observed in systems of quite different salt concentrations $10^{-6} molL^{-1} \leq c_S \leq 10^{-2} molL^{-1}$ [6]. The observed behaviour stays theoretically unexplained. However, in other studies we observed the mobility to start with a plateau, but then to decrease [7, 8]. In the latter case, the onset of the decrease coincides with the onset of counter ion dominance, i.e. when the counter-ions of the charged particles start to dominate the small ion population [9]. This was reproduced in computer simulations [8] and is theoretically understood in terms of the electrolyte concentration dependence of the zeta potential [9]. Using a novel scheme for correcting multiple scattering contaminated Doppler spectra [10] and the possibility to simultaneously characterize both electrophoretic and electro-osmotic mobilities [11], we now measured particle mobilities over an extended concentration range. We observed that electro-phoretic mobilities first increase, the reach the plateau values and, finally, decrease. Interestingly, osmotic mobilities do not show any pronounced dependence on the particle concentration.

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CO4 Jamming and shear thickening in a centrifuge

BRADLEY, Joe (University of Edinburgh); ROYER, John (University of Edinburgh)

In colloid and suspension science, it is not uncommon to assume that the sediment in a well-centrifuged sample at least approximates random close packing (RCP), and centrifugation is sometimes used as a calibration method to prepare samples at given volume fractions. We investigate sedimentation of a non-Brownian shear thickening suspension, where the shear rheology is controlled by two limiting packing densities: ϕ_{RCP} where the low-stress (frictionless) viscosity diverges, and $\phi_m < \phi_{RCP}$ where the high-stress (frictional) viscosity diverges. Varying both the initial volume fraction of the dispersed particles and the effective gravity under centrifugation, we show that this shear thickening behaviour also controls the final packing density of the sediment. Lower initial concentrations and higher effective gravity result in less dense sediments, suggesting the formation of frictional contacts between sedimenting particles above a critical pressure, analogous to the critical stress for the onset of thickening in shear rheology. In this thickened state, the sediment becomes jammed much closer to ϕ_m, analogous to random loose packing for frictional particles, before reaching the random close packed state for friction-less particles. Given the ubiquity of shear thickening in many diverse types of suspensions, these results indicate that random close packing is more likely the exception rather the rule in samples centrifuged at high speeds. These results also suggest the potential for centrifugation as a high-throughput method to measure ϕ_m and ϕ_{RCP} without relying on rheometric techniques.

CO5 Fluctuating stresses and the intrinsic viscosity of colloids

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PALANISAMY, Duraivelan (University of Twente)

Brownian Dynamics is a standard tool to study colloidal suspensions in the Stokesian flow regime. The solvent is treated implicitly, as the source of both hydrodynamic friction and stochastic forces obeying the fluctuation-dissipation theorem. Even though this formalism has been used extensively, and forms the basis of many theoretical studies on colloids, we show that it does not predict the correct intrinsic viscosity. A straight forward Green-Kubo calculation of the intrinsic viscosity of a quiescent dilute solution of spherical particles yields the surprising result $[\eta] = 0$, in marked contrast to Einstein's well-known $[\eta] = 5/2$. We propose a remedy to this problem, by introducing an extended fluctuation-dissipation theorem including Brownian stresses. Evaluating the correlations between these stresses and the Brownian forces gives rise to a further unexpected stress contribution. Using a recently developed rotational Brownian dynamics scheme, we also present a numerical rheology study confirming the validity of the proposed modifications to the Brownian formalism. We show that agreement is restored between the viscosities of quiescent and slowly sheared colloidal suspensions, for a range of body shapes, and that the linear rheology extracted from Brownian simulations now agrees with previous theories.

CO6 Stability of a particle-laden film falling down an incline

DHAS, Darish Jeswin (Indian Institute of Technology Madras); Roy, Anubhab (Indian Institute of Technology Madras)

The stability of particle-laden thin film falling down an incline is investigated using a nonlinear wave theory and a linear stability analysis. In absence of particles, the stability of a gravity-driven thin film has been extensively studied. Yih (1963) in his pioneering study carried out a linear stability analysis and identified a long wavelength instability in a falling film. Subsequently Benney (1966) performed an expansion in wave amplitude and derived a nonlinear wave equation describing the evolution of the film height that reproduced the linear stability findings as a limiting case. The presence of particles alters the rheology of the fluid with the non-uniformity of particle concentration altering the local shear viscosity leading to a coupling with the momentum balance. Using a Benney-like amplitude expansion, a set of coupled nonlinear equations are derived describing the evolution of film height and particle concentration. The modified Benney equation is solved numerically and the threshold of instability is calculated. On linearizing the governing equations, a generalized Orr-Sommerfeld system of equations is derived. The predictions of linear stability analysis are then compared with the results from nonlinear long wave theory.

CO7 Watching the Birth of a Binary Icosahedral Quasicrystal of Hard Spheres

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The binary $MgCu_2$ Laves phase consists of two sublattices, one diamond and one pyrochlore, that display wide photonic bandgaps at low refractive index contrasts. The three Laves structures, $MgCu_2$, $MgNi_2$, $MgZn_2$, can be assembled in a binary hard-sphere mixture. As all three Laves structures pack with the same density, the free-energy difference between them is very small. However, the $MgZn_2$ Laves phase is the most stable phase, and unfortunately not the aimed $MgCu_2$ phase. Here, we show by simulations that thousands of these particles in a spherical confinement spontaneously crystallize into a 3D icosahedral binary quasicrystal. The diffraction pattern of this quasicrystal shows all the characteristics of an icosahedral quasicrystal — it exhibits five-fold, two-fold, and three-fold orientational symmetry, as well as pentagons of which the sizes are inflated by powers of the golden mean. In addition, we observe that the icosahedral quasicrystal consists of concentric shells of either small or large spheres, and we identified the icosahedral quasicrystal cluster as a Bergman cluster, which is a fundamental cluster often used in the classification of icosahedral quasicrystals. More surprisingly, the quasicrystal consists of twenty tetrahedral domains that predominantly consist of particles with a $MgCu_2$-like symmetry, whereas the edges of five neighbouring tetrahedral domains form a pentagonal tube that originates from the Bergman cluster, runs through the whole cluster, and ends at one of the twelve vertices with a five-fold symmetry on the surface of the quasicrystal cluster. Finally, we investigate one of the many open questions on icosahedral quasicrystals — Can we watch the birth of a icosahedral quasicrystal and how does it grow? Does the quasicrystal nucleate from a Bergman cluster and grow shell-by-shell? Or does crystallization start at the spherical interface? We find that that the quasicrystal forms via nucleation far away from the spherical interface and is induced by the pronounced layering of the fluid into concentric shells. The growth of the quasicrystal is directed along the pentagonal tubes. We corroborate our simulations with experiments on binary nanoparticles suspensions, and we indeed observe experimentally the formation of icosahedral quasicrystals induced by the spherical confinement of slowly drying emulsion droplets. We thus find that a binary mixture of hard spheres, that crystallizes into the $MgZn_2$ Laves phase in bulk, spontaneously forms an icosahedral quasicrystal composed of tetrahedral domains with $MgCu_2$-like symmetry in a spherical confinement. Our simulations show for the first time the birth of an icosahedral quasicrystal of hard spheres.

CO8 Rheology and phase behaviour of multi-responsive soft microgels

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Soft colloids have attracted great interest in the last few years for both theoretical implications and technological applications. Indeed, they are very good model systems for understanding the general problem of dynamic arrest, since their larger tunability with respect to atomic and molecular systems leads to complex phase behaviours. Among them multi-responsive microgels, colloidal suspensions of micro- or nanometre-sized hydrogel particles, are very intriguing systems due to their high responsiveness to external stimuli such as pH, temperature, electric field, ionic strenght, solvent, external stress or light pulses. One of the most studied microgel is the thermo-responsive poly(N-isopropylacrylamide) (PNIPAM) whose thermo-responsiveness is strongly related to the temperature induced coil-to-globule transition of the NIPAM polymer. At room temperature indeed, PNIPAM microgels are in a swollen state, due to the polymer hydrophilicity that leads to dominant polymer-solvent interactions and to the retention of a great amount of water. By increasing temperature, across the volume phase transition (VPT) (T 305K), the polymer becomes hydrophobic, polymer-polymer interactions become stronger, water is completely expelled and particles reach a shrunken state. In this work we study an Interpenetrating Polymer Network (IPN) microgel composed of PNIPAM and a pH-responsive polymer as poly(acrylic acid) (PAAc) [1,2]. The IPN preserves the same VPT temperature of pure PNIPAM microgel and permits to control polymer/polymer and polymer/solvent interactions through pH [3]. Here we report rheological and differential scanning calorimetry measurements on aqueous suspensions of PNIPAM-PAAc microgels as a function of temperature, weight concentration and PAAc content. The frequency dependent linear viscoelastic properties across the typical swollen-shrunken volume phase transition are deeply investigated [4] and a preliminary phase diagram is reported.

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CO9 Probing the interface of colloidal interaction; experimentally examining the double layer overlap.

FRENCH Joseph (University of Edinburgh); ROYER, John (University of Edinburgh); VASILEIOS, Koutsos (Univeristy of Edinburgh); POON, Wilson (University of Edinburgh)

The repulsion between two charged surfaces traditionally relies on the Deryagin?Landau? Verwey?Overbeek (DLVO) potential to explain interactions across micrometer length scale. However, at lengths below the Debye length a new algebraic theory has been put forward to explain the relationship between the disjoining pressure and the interplate distance. In this poster, this theory is applied to experimentally derived force-distance curves in order to explore interacting silica-silica surfaces at lengths below the debye length, within the double layer overlap. This could potentially explain close range colloidal interactions in terms of surface charges and ionic strength.

CO10 Compartmentalisation of tiny depletants in crowded discotics

GONZÁLEZ GARCÍA, Álvaro (Eindhoven University of Technology); TUINIER, Remco (Eindhoven University of Technology); CUETOS, Alejandro (Universidad Pablo Olavide)

Whenever dispersed colloidal particles are mixed with non-adsorbing species, an indirect, entropy-driven attraction between the colloids emerges. The range of the resulting depletion interaction is set via the size of the so-called depletant. Here, we study the effects of adding tiny depletants to a discotic system. This gives rise to a low-density columnar phase (C_1) coexisting with a denser one (C_2). Theoretically, we account for the volume available for depletants in the columnar state on geometrical grounds. The performed direct coexistence Monte Carlo simulations enable to determine the C_1–C_2 equilibria and its stability. Tie-lines from theory and simulations are remarkably close. Deviations can be explained from different mesogenic colloids considered in theory and simulations. It becomes clear that an accurate account of the compartmentalization of these tiny depletant over the different high-density phases is key to understanding the coexistence at hand. In the lower-density columnar phase (C_1) depletants are present between the flat faces of the discotics, as opposed to the denser phase (C_2). Consequently, the C_1–C_2 coexistence is driven by the depletant partitioning along the columns. Only hard (repulsive) colloid?colloid and depletant?colloid interactions are considered: entropy suffices to explain crystalline-like coexistences at high colloidal densities, where depletants compartmentalise among the pockets of the colloidal phases. Our results provide a fundamental understanding on partitioning effects in highly concentrated and size-asymmetric environments, relevant in biological systems.

CO11 Investigation of fluid-fluid and solid-solid phase separation of symmetric non-additive hard spheres at high density.

GOZDZ, Wojciech (Institute of Physical Chemistry Polish Academy of Sciences)

We have calculated the values of the critical packing fractions for the mixtures of symmetric non-additive hard spheres at high densities for small values of the non-additivity parameter. The calculations have been performed for solid-solid and fluid-fluid demixing transition. A cluster algorithm for Monte Carlo simulations in a semigrand ensemble was used and the waste recycling method was applied to improve the accuracy of the calculations. The finite size scaling analysis was employed to compute the critical packing fractions for infinite systems with high accuracy.

CO12 From protein phase behavior to second virial coefficient

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We experimentally determined the phase behaviour and the interactions of protein (lysozyme) solutions under conditions favouring protein crystallization and metastable gas-liquid phase separation [1-3]. The phase behaviour as well as the interactions show striking similarities to those of colloids with short-ranged attractions. In particular, we find that the rescaled metastable gas-liquid binodals of protein solutions can be mapped onto those of square-well fluids [4]. Despite their much more complex interactions, protein solutions hence appear to also follow the extended law of corresponding states [5]. Moreover, we exploit this extended law of corresponding states in order to infer the second virial coefficient B2 from the phase behaviour, namely, the cloud-point temperature [6]. This determination of B2 yields values that quantitatively agree with results of static light scattering experiments.

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CO13 Grain Growth in Impurity-Doped Two-Dimensional Colloidal Hard Sphere Crystals

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Coarsening corresponds to the non-equilibrium relaxation in a quenched system [1]. The resulting domain growth is often driven by a reduction of inter-domain length, due to a minimisation of interfacial energy. In crystals, these domains are grains: crystalline regions in which all particles exhibit the same crystal orientation with respect to their neighbours. Grain growth is important to study, as the microscopic grain size sensitively affects the macroscopic properties of materials such as metals and ceramics [2]. The addition of impurities can impede grain growth, so careful doping can be applied to control the mechanical properties of polycrystalline materials.

Here, we examine the crystallisation and grain growth in impurity-doped two-dimensional colloidal crystals. We achieve this by creating a monolayer of binary colloidal hard spheres, with the smaller particles forming the grains and the large ones acting as impurities. We prepare polycrystalline systems with different concentrations of impurities, and follow the evolution of the system using video-microscopy over thousands of Brownian times. We analyse the initial crystallisation and the subsequent grain growth by monitoring the fraction of crystalline particles, the total grain boundary length and the grain boundary character distributions. In contrast to grain growth in monodisperse, i.e. impurity-free, two-dimensional colloidal crystals [3], we find a combination of crystallisation and grain growth in systems with low impurity concentrations, while crystallisation is arrested and grain growth absent at high impurity concentrations.

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CO14 Rotational and translational diffusion of elliptical particles

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Confocal microscopy is a well established method for real space imaging of colloidal particle diffusion. Hitherto, most of the experiments were focusing on monitoring the translational movement of spherical particles. By contrast, the rotational dynamics of anisotropic colloids have so far received only little attention. To be able to simultaneously follow the translational and rotational diffusion of elliptical colloidal particles in dilute suspensions, we developed PMMA/PMMA core-/shell-colloids in which core and shell were labelled with different fluorescent dyes. The particles contain cross-linked, spherical cores, whereas the shells are transformed into an ellipsoidal shape by stretching the particles in a PDMS matrix. With this procedure it is possible to obtain monodisperse ellipsoidal shaped particles with specific aspect ratios. We studied the translational and rotational diffusion of elliptical particles with different aspect ratios. A dedicated algorithm was used to derive spatio-temporal trajectories from 3D confocal microscopy images. The diffusion data obtained confirm predictions from hydrodynamic theory [2].

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CO15 Shear-switched Bistability in Binary Systems

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Particulate suspensions consisting of solid particles suspended in a fluid medium are widely involved in industry. Among the various industrial suspensions, one of the most common type is suspensions containing particles suspended in a yielding background with yield stress arising from the attractions between colloidal particles, e.g. concretes, toothpastes and battery electrodes. Such systems can be viewed as non-sticky particles embedded in a colloidal gel, and the polydispersity makes their properties far more complex than single-component systems. In order to predict their flow behaviours in practical situations, there is a compelling need for more realistic model systems in the lab. Here we develop a model system composed of non-Brownian repulsive particles suspended in a colloidal gel of smaller attractive particles. Using rheo-confocal microscopy, we find that two structural states can be induced by different shears in one sample: homogeneous state (induced by high shear) and phase-separated state (induced by medium shear). The two states differ in both microstructures and mechanical properties, and the transition between them is reversible under shear, i.e. the system can be switched to the desired state by simply imposing corresponding shear rate. The two structural states offer the binary model system a complex history-dependence, and our results have a strong implication for material design and industrial formulations.

CO16 Impact of highly concentrated suspension drops

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We study the deformation of a suspension drop, made of non-Brownian spherical beads suspended in a Newtonian liquid, upon impact onto a flat solid surface.

We focus on the range of large particle volume fractions (typically 50% to 64%), extending both below and above the critical volume fraction ϕ_c, at which the steady viscosity diverges [Boyer et al, 2011], and which also separates the dilative and contractive responses of a sheared bead pile (Reynolds dilatancy).

Over this range, the drop deformation, as quantified by the diameter of the deformed drop relative to its initial diameter, shows two different trends. For fixed impact conditions (suspending liquid viscosity η, impact speed V, bead size d) and at moderate ϕ, the deformation decreases with increasing ϕ, in agreement with the effective Newtonian rheology of the suspension. However, around $\phi \approx 55\%$, deformation begins to deviate from the Newtonian behavior, and finally saturates around $\phi \approx 60\%$.

We will discuss how the deviation from the Newtonian behavior and the deformation plateau at high ϕ depend on the suspending liquid viscosity η, the impact speed V, and the bead size d.

CO17 Pore cross talk in colloidal filtration studied by nanofluidic chips

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The clogging of a membrane by small particles is crucial in several industrial processes, e.g. for the filtration of water. The phenomenon is usually studied at the global (system) scale: kinetics of ‘filtration cake’ growth, reversibility. Recently, model microfluidic systems have been proposed to elucidate elementary events at the pore scale thanks to simplified configurations [1]. However, the situation of Brownian particles and sub-micrometric pores has hardly been assessed until now, in spite of its relevance for real devices: microorganisms? removal is for instance usually done by 0.22 m diameter holes. In this context, we perform experiments where model sub-micrometric pores are clogged using a monodisperse Brownian suspension. We use simple geometries connecting two microchannels (etched in silicon) through an array of nanoslits obtained by clean-room microfabrication, to get insight into the mechanisms of clogging at the pore scale. We measure a coupling between neighbouring pores concerning the growth rate of clogs during the filtration process. The growth rate of a clog formed by particles at a pore entrance systematically increases with the number of already saturated (entirely clogged) pores, indicating that there is an interaction, or ‘cross-talk’, between the pores. This observation is interpreted based on a phenomenological model, stating that a diffusive redistribution of particles occurs along the membrane, from clogged to free pores [2]. This one-dimensional model could be extended to two-dimensional membranes. Results that are more preliminary concern the role of a cross-flow on the saturation size of clogs, evidencing a competition erosion/drag. Information on the structure of the clog is also obtained from the way it disintegrates when the flow is stopped after clogging.

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CO18 Unifying viscous and inertia regimes of discontinuous shear thickening suspensions

Junhao Dong (Lund University, Sweden); Trulsson, Martin (Lund University, Sweden)

We have shown previously that fraction of friction contact χ_f is a key parameter to characterise the rheology of shear thickening dense suspensions besides viscous number J. With binary model (*i.e.* binary mixture of frictional and frictionless particles), we are able to control values of χ_f and investigate the dependence of constitution laws on χ_f. Expressions of constitution laws for relative viscosity $\eta/\eta_f = g(\phi, \chi_f)$, packing fraction $\phi(J, \chi_f)$ and number of contacts $Z(J, \chi_f)$ are derived and compared with simulation data, which shows that derived functions manage to well describe simulation results.

Furthermore, rheology of granular flow, which is characterised by inertia number I, has been shown to be able to be unified with dense suspensions with proper scaling factor between I and J. Again with binary model, we show here that macroscopic properties $\eta/(\dot{\gamma}\rho d^2)$ and ϕ of granular flows can collapse with corresponding data from dense suspensions with scaling J and I^2. While for collapsing Z, the scaling is J and I^n with n being χ_f-dependent, and $n = 2$ for $\chi_f = 1$ and $n = 1$ for $\chi_f = 0$. Constitution laws for granular flows are then be derived from the ones for dense suspensions with proper adjusting parameters.

These expressions are then used to predict flow behaviour of dense suspensions and granular flows using Critical Load Model (CLM), a model usually used to reproduce discontinuous shear thickening behaviour (DST). The predictions are in good agreement with simulation results. Basing on these, we combine J and I and construct new dimensionless parameters, which are used to describe the transition from viscous to inertia regimes (*i.e.* suspensions with finite Stokes number), and validate the equations with numerical results. Finally, we further explore parameter space and show that various flow curves can be generated with different combination of shear protocols, threshold forces, viscous and inertia numbers.

CO19 Self-consistent multi-scale simulation of colloidal mixtures

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Analysis of coarse-grained models is useful for understanding the properties of many soft matter systems. We consider colloidal systems that consist of mixtures of large and small particles, in which the small particles mediate a depletion interaction between the large ones. In such systems, it is straightforward to derive a coarse-grained model with pairwise interactions among the large particles. However, this coarse-grained model is usually not an exact representation of the fully-interacting mixture (except for some classes of Asakura-Oosawa model).

We present a numerical method for exact computation of properties of these colloidal mixtures. We use the coarse-grained model to make a first-order estimate of the relevant properties, and then we compute correction factors that allow us to estimate exactly the properties of the fully-interacting mixture. The correction factors are obtained using Jarzynski's equality to obtain unbiased estimates of the free energy of the small particles. By exploiting mathematical results for multi-level statistical estimators, we show how this can lead to efficient numerical performance.

We illustrate the method by analysing the liquid-vapour critical point in Asakura-Oosawa systems for which three-body and many-body interactions are significant. We consider a coarse-grained model that neglects three- and many-body interactions. We show that our method can quantify the errors associated with this approximation, and recover the exact result for the full system. We will also show preliminary results for hard-sphere mixtures, where many-body interactions have significant effects. We discuss future directions, including a generalisation of the method to other soft matter systems.

CO20 Self-assembly and thermal conductivity of nanofluid using Janus or homogeneous nanoparticles

KOBAYASHI, Yusei (Kindai University); ARAI, Noriyoshi (Kindai University)

Nanofluids are suspensions of nanoparticles (NPs), which exhibit remarkable thermal properties and therefore have many potential applications in electronics, engineering, biomedical, and optical fields. Before designing an application of nanofluidic devices, we need to understand the thermophysical properties of nanofluids, such as thermal conductivity, viscosity, and heat capacity. However, despite several decades of research effort, the detailed mechanism for the unusual thermophysical properties has not been completely clarified yet. Some of the studies conducted on nanofluids have delivered conflicting results and thus controlling and predicting the rheological and thermal physical properties of nanofluid is still challenging.

Here, the self-assembly of nanofluid is an important technique for controlling their rheological properties (e.g., viscosity and thermal conductivity). Self-assembly of nanofluid (nanoparticle) can spontaneously result in various morphologies depending on the volume fraction of nanoparticle, the chemical nature of nanoparticle surface, solvent type, and the temperature, among other physical conditions. Hence, the prediction and control of the self-assembly of colloidal nanoparticles is very important and constitute a useful process in materials chemistry and engineering.

Previous studies have already been reported on the thermal properties of nanofluids. However, the mechanism of thermal properties has not been clarified so far. We performed molecular simulations to investigate the thermal properties of nanofluids. Here, we attempt to investigate the influence of the addition agent (nanoparticles) properties on the thermal conductivity. Three distinct types of nanoparticles were considered: hydrophobic (HO), hydrophilic (HI), and Janus. We observed diverse self-assembled structures between the different nanoparticle designs. Moreover, we found that the thermal conductivity behavior depends on the self-assembled phase and the chemical nature of the nanoparticles surface. For examples, when hydrophobic NPs are added to a nanofluid, they only form one large cluster because they do not prefer to be in contact with water molecules. Hence, an increment in the thermal conductivity of the nanofluid added with HO NPs was observed. On the contrary, the cluster size of Janus NPs was limited because of their limited HO superficial areas (attractive domains). Hence, an increment in the enhancement ratio of thermal conductivity was not observed even when the volume fraction of the NPs was increased. Thus, our results demonstrate that the cluster size of NPs is the key factor for thermal conductivity enhancement.

Our simulation provides new insights on how a change in the chemical surface design of NPs influences their self-assembly and the thermal conductivity behavior of nanofluids, which constitute novel systems that may find applications in heat transfer including engine cooling/vehicle thermal management, hybrid-powered engines, and fuel cells.

CO21 Shape controls polarization: Self-organization into ferroelectric and antiferroelectric crystals by shape-anisotropic particles

Kyohei Takae (Institute of Industrial Science, University of Tokyo); Hajime Tanaka (Institute of Industrial Science, University of Tokyo)

Ferroelectricity and antiferroelectricity are widely seen in various types of condensed matter and are of technological significance not only due to their electrical switchability but also due to intriguing cross-coupling effects such as electromechanical effects. The control of the two types of polarization ordering has practically been made by changing the ionic radius of a constituent atom or externally applying strain for inorganic crystals and by changing the shape of a molecule for organic crystals. However, the basic physical principle behind such controllability involving structural organization is still unknown. By using a simple particle model with strong coupling between polarization ordering and structural ordering [1], here we show that energetic frustration between the two types of anisotropic interactions, dipolar and steric interactions, is a key to control not only the phase transition but also the coupling between polarization and strain [2]. By utilizing this coupling, we also realize electric/mechanical switching between ferroelectric and antiferroelectric states.

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CO22 On the brownian and precessional motion of dense ellipsoidal colloids

LAGANAPAN, Aleena (University of Konstanz); FUCHS, Matthias

Hard colloidal ellipsoids are an interesting model system. First, the interactions and dynamics of hard ellipsoids can be described theoretically thus allowing us to minimize the number of assumptions and unknown variables in the model. Second, while the deviation from the hard-sphere geometry is small, the system already provides additional rotational degrees of freedom, which can exhibit a wide range of new properties, such as liquid crystalline order, that one can explore.

Our goal is to study the dynamics of a system of colloidal hard ellipsoids in the context of glass transition using an event-driven Brownian dynamics model. To this end, we develop an algorithm following the models proposed by Donev (2005) [1] and De Michele (2007) [2] for event-driven molecular dynamics. In contrast to these existing models, we further expand our work by incorporating brownian and precessional motion.

We benchmark our model by comparing our measured structural and transport properties, such as pair-correlation functions, mean-squared displacements and angular correlations, with experimental results of Roller et al. (2018) [3]. We also demonstrate that our model can be used to gain insight to the effects of (i) brownian motion, (ii) polydispersity and (iii) non-isotropic moments of inertia, to the behaviour of dense suspensions of ellipsoids. We expect this research to contribute to debates on nematic and orientational glass transition.

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CO23 Anomalous Dynamics of Concentrated Silica-PNIPAm Nanogels

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Poly(N-isopropylacrylamide) (PNIPAm) nanogels undergo a reversible volume phase transition (VPT) in water at a lower critical solution temperature (LCST) around 32°C, which results in a rapid collapse of the particle volume by increasing the temperature. Beside technical and medical applications, it has become a frequently studied system in soft matter research as a model system to probe the specific phase behavior of soft colloids. Via x-ray photon correlation spectroscopy (XPCS) and small angle x-ray scattering (SAXS) we investigate the structure and dynamics of highly concentrated PNIPAm core-shell nanogels around the LCST below the radiation damage threshold. Here we studied the dynamics and interaction of the highly concentrated colloids ($w = 14.6$ wt%) as a function of temperature around the LCST as well as the modifications due to their reversible VPT. Upon heating from room temperature to45°C we found three dynamical regimes: At low temperatures the colloids show a sub-diffusive, polymer driven dynamical behavior. Around the LCST the relaxation time decreases rapidly. For $T > 37$°C the dynamics slow down by more than three orders of magnitude and the particle motion becomes hyper-diffusive. Together with the static data, where we found indications of a transition from repulsive to attractive forces during the VPT, our results suggest a transition from a polymer-dominated liquid below the LCST to a jammed state at high temperatures and volume fractions.

CO24 Critcality at finite deformation rates in sheared yield stress materials under external excitations

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The flow properties of soft disordered solids such as emulsions, foams, granular materials and others are characterized by critical features at the yielding transition (limit of vanishing shear rates) and, under certain circumstances, by a regime of coexistence between regions flowing at different shear rates (bands). The emergence of critical dynamics at finite shear rate is however still poorly understood and has only been addressed in the case of vibrated frictional granular materials in a recent work [Wortel et al., PRL 2016] where an external mechanical vibration induces a transition from a non-monotonic to a monotonic flow curve, accompanied by critical-like fluctuations of the macroscopic shear rate.

In this study we investigate the role of an external agitation in a mesoscale elasto-plastic model for the flow of dense disordered materials exhibiting a shear banding instability. We evidence a transition from phase separated to homogeneous flow accompanied by critical-like fluctuations of the macroscopic shear rate. The scaling of fluctuations is found to be consistent with the scaling of the macroscopic flow curve across the transition. We also find that some of the critical exponents characterizing this dynamical phase transition to be in agreement with experimental observations. Altogether, this suggests a possible generic mechanism for the emergence of critical features when self-fluidization mechanisms associated to shear weakening compete with an external source of noise.

CO25 Neural networks for nucleation

LEONI, Fabio (School of Mathematics, University of Bristol, UK); RUSSO, John (School of Mathematics, University of Bristol, UK)

We study the properties of the critical nucleus forming during spontaneous homogeneous nucleation in hard spheres and many-body interaction systems, such as the mW model. We analyse the structure of the nucleus following a neural network approach. Introducing a new order parameter we find results at variance with those obtained using common widespread methods in the literature.

CO26 Microfluidic Flow of Colloid-Liquid Crystal Composite Materials

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Liquid crystals are fascinating states of matter with properties between those of conventional crystalline solids and simple liquid. They combine the intrinsic fluidity of liquids with long-range orientational order, which couples with the flow and induces novel effects that do not exist in isotropic Newtonian fluids, such as backflow, anisotropic stresses and multiple viscosities. A wealth of literature on bulk hydrodynamics of liquid crystals exists, but the study of even the simplest liquid crystals, the nematic phase, in microfluidic confinement is still relatively new and has been so far predominantly dealing with pure phases [1].

Colloidal particles in liquid crystals exhibit a very different behaviour to that observed in an isotropic medium [2]. This arise because of the induced elastic stresses that are exerted due to the interaction of the liquid crystal with the particle surface. Interfaces introduce also topological defects and domains where the liquid crystalline order is strongly suppressed [3]. This arises due to the incompatibility of the local anchoring conditions on the particle surface with the long-range order of the liquid crystal. Studies of particles in nematics have generally focused on how the molecules reorder around a single particle that is held in position. More recent experimental studies have focused on the dynamic behaviour of finite sized suspended colloidal particles in a nematic-fluid flow [4].

We present results of large-scale lattice-Boltzmann simulations of a colloid - liquid crystal composite material in Poiseuille flow. The colloid volume fractions we investigated range from a few percent up to about 40%, covering the full scale of possible morphologies from single isolated particles to clustering particles that are surrounded by a percolating defect network. Depending on volume fraction, pressure gradient and anchoring conditions we observe intriguing effects that have not been reported so far. This includes the reorientation of the local defect network around the colloidal particles at low colloid densities, states which feature negative mobilities among a significant fraction of the suspended particles at larger colloid volume fractions and low flow velocities as well as a percolating network of topological defects that seem to act as low-viscosity conduits for the flow.

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CO27 Short-time diffusive dynamics of proteins in a naturally crowded environment

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In living cells, 10-40% of the intracellular fluid volume is occupied by macromolecules. This condition of macromolecular crowding influences reaction rates and signal transduction. We investigate the effect of crowding on the short-time tracer diffusion of model proteins on the nanometer length and (sub-) nanosecond timescales both experimentally and with the aid of computer simulations. Experimentally, we dissolve polyclonal immunoglobulin (Ig) antibody proteins of natural isotopic abundance as tracers in perdeuterated Escherichia coli cell lysate as crowder to mimic a biological environment and at the same time optimize the sensitivity for the tracers using incoherent quasi-elastic neutron scattering. We subsequently compare the ensemble-averaged dynamics of Ig in lysate to the dynamics of Ig in pure water as a function of concentration. In both cases, remarkably, the diffusion of Ig only depends on the total macromolecular volume fraction ? in the sample, within the experimental accuracy. To shed light on how polydispersity affects the short-time self-diffusion of proteins in crowded environments, we perform computer simulations which have proven to provide accurate information on the diffusion of proteins in crowed environments and to interpret and rationalize neutron scattering experiments. Because of the times scales and the relevance of hydrodynamic interactions (HI) in our experiments, we perform simulations based on Stokesian Dynamics in which HI are considered explicitly and short-time properties can be calculated. In our approach, the lysate polydisperse system is modeled using hard spheres. We demonstrate an intricate dependency between the diffusion of a tracer on the crowder composition, specifically on the ensemble effective radius, $R_{\mathrm{eff}} = \langle R_i^3 \rangle^{1/3}$. For tracers with a radius close to R_{eff} , the tracer diffusion is similar to that of a monodisperse system, whereas deviations are observed for significantly different tracer radii. Notably, the hydrodynamic radius of Ig is close to the lysate effective radius, which explains the surprising insensitivity to the polydispersity observed in the experiments. The simulation results further show that polydispersity slows down larger macromolecules more effectively than smaller ones even at nanosecond timescales. This has obvious implications for the functioning of the cellular machinery. Our simulations also confirms the predictive power, on the nanosecond timescale, of coarse-grained molecular dynamics simulations.

CO28 Nematic and Triatic phases of hard isosceles triangles: One component fluid and binary mixtures

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Phase transitions in two-dimensional liquid crystals have received recent attention due to the possibility to reduce the dimension of colloidal systems by strong confinement. Also, vibrated granular monolayers of hard anisotropic particles are examples of experimental realizations of two-dimensional systems forming liquid-crystal textures. Most of studies were centered on hard rods. Here we propose the triangular geometry as a shape driving phase transitions between orientationally ordered phases with novel symmetries. We formulate the scaled particle theory for a mixture of hard isosceles triangles and calculate different phase diagrams for the one-component fluid and binary mixtures. The fluid of hard triangles exhibits a complex phase behavior: (i) the presence of a triatic phase with sixfold symmetry (also found in recent MC simulations of equilateral triangles), (ii) the isotropic-uniaxial nematic transition is of first order for certain ranges of aspect ratios, and (iii) the one-component system exhibits nematic-nematic transitions ending in critical points. We found the triatic phase to be stable not only for equilateral triangles but also for triangles of similar aspect ratios. We focus the study of binary mixtures on the case of symmetric mixtures: equal particle areas with aspect ratios (κ_i) symmetric with respect to the equilateral one: $\kappa_1\kappa_2 = 3$. For these mixtures we found, aside from first-order isotropic-nematic and nematic-nematic transitions (the latter ending in a critical point): (i) A region of triatic phase stability even for mixtures made of particles that do not form this phase at the one-component limit, and (ii) the presence of a Landau point at which two triatic-nematic first-order transitions and a nematic-nematic demixing transition coalesce. This phase behavior is analog to that of a symmetric three-dimensional mixture of rods and plates.

CO29 A constraints-based approach to tuning the rheology of a non-model suspension

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Granular suspensions can exhibit a range of rheological behaviours depending on the particle-particle interactions, ranging from shear thickening in repulsive (well-stabilised) particles to shear thinning and the development of a finite yield stress with adhesive particles. Recently, a mean-field model has been proposed which can analytically capture this range of behaviour based on the constraints imposed by frictional and/or adhesive particle contacts. This model was initially developed with idealised nearly-spherical, nearly-monodisperse particles in mind, however such suspensions are rarely encountered in actual industrial practice. We examine the rheology of suspensions of ground quartz flour suspended in aqueous glycerol/water solutions, adding an anionic surfactant (sodium dodecyl sulfate) to vary the particle interactions from attractive to repulsive. These quartz flour suspensions strongly deviate from typical model suspensions, comprised of highly-angular and highly-polydisperse particles. However, despite using these ?messy? particles, we find that we can still apply the same constraints-based mean-field model to fit our experimental rheology, highlighting the utility and generality of such an approach.

CO30 Correlated diffusion of colloidal particles in two-dimensional random confinement

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Correlated diffusion of tracer particles embedded in a quasi two-dimensional model porous medium made of a random matrix of large colloidal particles sandwiched between two glass plates is investigated. We use the two-point mean squared displacement (2P-MSD), a measure of the coupled motion of particle pairs. A range of matrix porosities were achieved by pressing suspensions of small and large colloids between two glass slides such that the large particles are stuck between the slides, forming the matrix, while the small particles are mobile. We find that at all matrix packing fractions the 2P-MSD has the same form as that of particles confined solely between two plates ? namely it decays with the interparticle distance r as $1/r^2$. However, the magnitude of the hydrodynamic coupling decreases with increasing matrix packing fraction. In addition, there is anomalous time dependence at high matrix packing fractions, with sub-diffusive behaviour even at short lag times, which is related to a decrease in the mean pore size.

CO31 Complex Formulations Drying on Complex Substrates

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Drying of droplets containing colloidal particles is critical to many industrial practices, such as inkjet printing, microelectronics and pesticide spraying on plant leaves. For the latter, the deposit pattern can affect the uptake through the leaf. In the literature, one can find many examples of how different formulations affect drying, but little is known about how the surface texture affects the drying process and hence the dried deposit. Additionally from a fundamental point of view, many more interesting questions remain unanswered, such as: how does the microstructure relate to the substrate properties; how the wetting properties vary with the deposit coverage; and what is the most adequate microstructure for a certain application.

Different roughness length-scales have been explored experimentally, ranging from the size of the colloidal particles (microns), to the order of magnitude of the drop size (mm). An in-house Python code has been developed for the image analysis of the dried deposits, defining a parameter that relates the roughness of the substrate to the dried pattern. Furthermore, moving from PDMS to paraffin substrates provides a more similar surface to those in waxy leaves. This, along with exploring particle and droplet sizes comparable to those used for pesticide spraying, will help create a model system for crop care applications.

CO32 On the origin and evolution of depletion zone in coffee stains

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A colloidal droplet evaporating on a solid substrate is a simple yet far-reaching scientific problem, owing to the rich and diverse fluid flow patterns generated within the droplet, which leads to the formation of a variety of self-assembled structures. A non-uniform ring-like deposit, termed as coffee-ring is a ubiquitous deposition pattern formed on evaporation of sessile colloidal droplets containing solid un-dissolved particles. Addition of surfactants to colloidal systems is known to modify the flow patterns responsible for the formation of coffee-rings, leading to the formation of uniform deposits [1]. Variation in the concentration of surfactant molecules along the interface of the droplet leads to surface tension driven Marangoni flows, which inhibits the build-up of particles near the periphery of the droplet stain and also leads to the formation of 'depletion zones' within the coffee-stains. However, due to their small size, in-situ optical imaging of surfactant molecules is impossible. This poses limitations in understanding the mechanism of formation and the growth kinetics of depletion zones. Here we employ sessile droplets containing a mixture of polystyrene particles and surface active pNIPAM microgels as model systems to investigate the origin and evolution of depletion zones. These colloidal scale particles can be easily observed under an optical microscope thereby enabling in-situ observations on sessile droplets. We show that the fluctuations in the PS particle concentration along the interface is responsible for the formation of depletion zones in the system [2]. The depletion zones begin to form during initial stages of evaporation and further widens non-linearly with time, during evaporation. The growth rate of depletion zone for droplets containing different concentrations of PS particles collapses onto a master curve on scaling with concentration and radius of the droplet. It is observed that the critical time at which the depletion zone just begin to form decreases with increase in the PS particle concentration inside the droplet. Further, the critical time correlates well with the time at which the PS particle concentration gradient is maximum along the water-vapour interface.

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CO33 Sub-Arrhenius diffusion in a binary colloidal system

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The molecular dynamics simulation of a binary colloidal system subjected to an external repulsive potential reveals that the attractive depletion interactions between the barrier and the larger particles help larger particles to diffuse faster than the smaller particles over the potential barrier at low temperatures. The smaller particles get localized in between the potential barriers indicating a dynamics similar to system undergoing a glass transition. The anomaly in self diffusion coefficients of both the species reveal that the diffusive dynamics of the larger particles exhibit sub-Arrhenius temperature dependence at low temperatures, which is unusual for a classical system; whereas smaller particles obey normal Arrhenius diffusion. The activation energy of larger particles is found to be temperature dependent and hence changes the effective barrier height accordingly; while that of smaller particles is temperature independent. The waiting time distribution of both the species of particles verifies the nature of dynamical properties of the system. This model, classical by construction, challenges the widespread belief that sub-Arrhenius behavior is an effect of quantum tunnel origin. However the dynamics approach towards the classical regime, i.e, the larger particles show super-Arrhenius diffusion, as the density increases.

CO34 Dynamics of protein dispersions with competing interactions: Theory, simulation and experiment

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The dynamics in dispersions of proteins with competing short-range attraction and long-range repulsion (SALR systems) such as in low-salinity lysozyme solutions has gained a lot of interest over the past years. SALR systems have a rich phase behavior, including equilibrium and non-equilibrium cluster phases We investigate the influence of protein clustering on the dynamics and structure in SALR dispersions, by combining a theoretical method where hydrodynamic interactions (HIs) are approximately included [1] with multiparticle collision (MPC) simulations accounting for the full many-particles HIs [2]. By this simulation-theory comparison, we establish the high accuracy of the theoretical method for calculating diffusion and viscosity properties of SALR systems in the dispersed-fluid phase region. We show that a cluster peak is present also in the hydrodynamic function characterizing the short-time dynamics, in accord with neutron spin echo results on lysozyme solutions [3]. The inter- and intra-clusters dynamics in the equilibrium cluster phase region is analyzed using MPC simulations [2] which reveal cluster shape changes and lifetimes strongly influenced by many-proteins HIs. We finally discuss the peculiar quasi-two-dimensional dynamics of SALR particles moving in a planar liquid interface [4].

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CO35 Another mechanism of diffusiophoresis with chemical reaction on a colloidal particle

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We propose a mechanism of diffusiophoresis for a charged particle undergoing a dissociation reaction on its surface in a weak electrolyte solution. A theoretical model is constructed to describe the dynamics of the particle and the surrounding solution of a weak electrolyte. Theoretical analysis and numerical simulations of the model reveal that phoretic motion of the particle emerges in response to a concentration gradient of electrolyte. Since in our model the solute is an undissociated (neutral) electrolyte, its concentration gradient cannot generate an electric field in the bulk far from the particle. However, the dissociation reaction with the solute yields asymmetric charge distribution, which gives rise to net force on the particle and leads to directional motion of the particle. Note that, unlike the Janus particle, the particle in our model does not possess any structure on the surface, but it can break the spherical symmetry of surface charge distribution due to the gradient of reactant (solute) concentration.

CO36 Extrusion of shear thickening suspensions: Variations in local solid concentrations

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In many industrial applications dense suspensions are forced from a reservoir through a constriction into a smaller pipe or channel. Dilution of suspensions is often encountered as they travel through a constriction. This phenomenon, commonly referred to as liquid migration (LM), can lead to catastrophic consequences. For example, LM can damage equipment and lead to product loss in extrusion-based manufacturing, and in medical applications, such as the injection of bone cement into a bone fracture, LM can be fatal. Despite these severe potential consequences, the mechanism(s) behind LM are poorly understood, making it difficult to predict and avoid the onset of LM. We investigate LM during the extrusion of well-characterised shear-thickening suspensions. We find that above the onset of LM, the extruded material maintains a steady concentration, ϕ_c, independent of time or initial concentration. This critical concentration depends on both the flow rate, Q, and the constriction (die) radius, rd, and at low flow rates collapses onto a universal function of Q/r_d^3, a characteristic shear rate in the die. Below ϕ_c no LM is observed, so that our collapsed data $\phi_c(Q/r_\mathrm{d}^3)$ defines a phase diagram for the onset of LM. We show that this phase boundary can be captured analytically by coupling the suspension shear rheology to a simplified 'suspension-balance' model describing the relative solid-liquid flow in response to local stress gradients [1]. Using x-ray imaging, we spatially map out variations in ϕ within the extruder. We observe the decrease in ϕ as the suspension enters the die. As the suspension upstream of the die supplies liquid to the dilating suspension, we observe an increase in ϕ in the suspensions directly surrounding the die, forming a dense zone, which grows throughout extrusion. We find suspension upstream of this dense zone is unaffected by LM.

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CO37 Asymmetric stress response in oscillatory shear of dense non-Brownian suspension studied by particle simulation

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Dense suspensions of non-Brownian spheres suspended in a Newtonian liquid are widely used in a variety of formulated products, such as paints, foods and cements. Understanding the transient rheology can be crucial in many of these applications. Using discrete element method simulations of particle dynamics taking into account of particle contact and lubrication interactions, we study the response of such suspensions under oscillatory shear, one of the most widely used method to study the transient shear rheology of materials. Our simulations reveal an asymmetric stress response between the forward and reverse half cycles under moderate amplitude oscillatory shear if the suspension has pre-sheared under steady-state simple shear. We find that this asymmetry is caused by the memory of the anisotropic contact network formed in pre-shear. This suggests that such memory effects should be taken into account to accurately predict the transient shear rheology of dense suspensions.

CO38 Translational and rotational dynamics of elliptical PMMA colloids

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Using 3D real-space imaging, the translational and rotational motion of spherical and elliptical PMMA/PMMA core-shell colloids can be studied. To date, nearly all real space imaging experiments of colloidal particle dynamics have been focused on monitoring translational motion of spherical particles. While the rotational dynamics of spherical particles have been studied in detail on a single particle level [1,2,3], the dynamics of anisotropic particle received only little attention due to difficulties in synthesis and sufficient 3D imaging and analysis techniques [4,5].

In this contribution, we present novel PMMA/PMMA core-shell ellipsoids with a spherical core and an elliptical shell labelled with different fluorescent dyes, which are well suited for 3D confocal microscopy [6,7]. The detection of each ellipsoid within the 3D image volume requires new image processing tools. To this end, we developed an algorithm able to detect each ellipsoid in position on subpixel accuracy and orientation within accuracy of 5 [7]. Using this approach, we experimentally study the structure and dynamics of a 3D system of monodisperse ellipsoids over a wide range of volume fractions. Our results provide insight into the phase behavior of ellipsoids in 3D and show both glass formation and nematic ordering.

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CO39 Confocal microscopy of optically trapped colloids

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Optical trapping of particles is an attractive method for active microrheology in colloidal suspensions. In combination with confocal microscopy it is a powerful tool for the investigation of colloidal dynamics under external fields. We present an experiment, in which a multifocal optical tweezer is combined with a confocal microscope. With this combination, independent 3D manipulation of single particles and the simultaneous 3D imaging of its environment becomes possible. We want to employ this setup to study dynamics of non-spherical colloids in dense suspensions.

A first focus of the experiment will be the determination of threshold forces, which are necessary to let a particle escape its cage in a glassy surrounding. The threshold forces are predicted to be approximately 40 fN for spheres with a diameter of 4m [1]. The particle?s environment and the particle itself will be imaged using confocal microscopy. Forces will be detected with backfocal plane interferometry. For our experiments we use core-shell particles with hard potentials. The host particles of the surrounding are core/shell PMMA/PMMA [2, 3] particles which are dyed with a fluorophore. By contrast, the tracer particles, which are manipulated with the optical tweezers are core/shell PMMA/PS particles. The tracer particles are dyed with a different fluorescent dye than the host particles such that they can be distinguished from the host particles. Both host and tracer particles can be of prolate ellipsoidal shape. The positions and orientations of each of the particles will be determined at each timestep (1 to 10 seconds) with a dedicated algorithm [4].

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CO40 Cornstarch suspensions in squeeze flow

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Suspensions of cornstarch are well known to present a shear-thickening behaviour, i.e. viscosity increases with the applied shear rate/stress [1]. Recent theories explaining shear-thickening behaviour attributed it to shear-induced frictional contacts between particles in suspensions [2]. Despite there are several works in literature regarding shear thickening from and experimental, simulation and a theoretical point of view; other kind of flows, like squeeze flow, have received much less attention. However, many industrial applications use highly-concentrated suspensions of particles in mixed flows with shear and extensional components.

The aim of this work is to study the rheological behavior of cornstarch suspensions in squeeze flow. Newtonian fluids are used to study the rheological relationship between normal force and gap. These results were fitted to theories for no-slip boundary conditions, obtaining viscosity values in a good agreement with literature. Results for cornstarch suspensions in squeeze flow showed a thickening behavior similarly to what is found in shear. Taking the second invariant of the rate-of-deformation tensor, the onset of the thickening was very similar to the shear-rate onset at each concentration. However, the jamming concentration was slightly lower, as predicted by molecular dynamic simulations for pure extensional flows [3]. Our results show that despite the complexity of the mixture of shear and extension strains in squeeze flow, the consequences of thickening can be understood in the same framework as for simple rheometric shear flow.

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CO41 Flow induced crystallization of penetrable particles

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For a system of Brownian particles interacting via a soft exponential potential we investigate the interaction between equilibrium crystallization and spatially varying shear flow. For thermodynamic state points within the liquid part of the phase diagram, but close to the crystallization phase boundary, we observe that imposing a Poiseuille flow can induce non-equilibrium crystalline ordering in regions of low shear gradient. The physical mechanism responsible for this phenomenon is shear induced particle migration, which causes particles to drift preferentially towards the center of the channel, thus increasing the local density in the channel center. The method employed is classical dynamical density functional theory.

CO42 How do halloysite nanoclays interact with negatively-charged polyelectrolytes?

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Recently nanotubes known as Halloysite nanoclays (HN) are attracting an ever growing interest as biocompatible versatile nanocarriers due to the possibility to load compound into their lumen or on their external surface [1]. This attractive property is connected to the presence of ionizable negative and positive groups on the outer and inner surface, respectively, in a large pH range. Several investigations show that a large variety of functional molecules and charged biopolymers can be efficiently loaded into the lumen and used for applications ranging from drug delivery to nanocomposite biomaterials [2,3]. Nonetheless the interesting contributions to the design, preparation, and characterization of a new soft hybrid nanomaterial, a deep understanding of the mechanism of interaction between HN nanoclays and charged polyelectrolyte is still lacking.

In this study, we propose to investigate the interaction between negatively-charged polyelectrolytes and HN nanoclays by an experimental approach based on dynamic light scattering, electrophoresys, Electron and Atomic Force microscopy and spectroscopic techniques. Calf thymus DNA and a linear flexible polyelectrolyte, sodium polyacrylate (NaPA) in different molecular weights, have been chosen as model polyanions with different stiffness and length. At the best of our knowledge, DNA was never loaded in the lumen of HN and in only one example, DNA is used to functionalize the external surface of HN through ball-milling process [4]. As DNA is a negative polyelectrolyte, how it can interact with negative external surface of HN is still an open issue. Moreover, the spontaneous loading into the lumen is also slowed down or hindered by entropic and osmotic reasons, while current methods force macromolecules loading by employ vacuum the capillary action induced by vacuum suction of air molecules trapped inside the lumen. Our results give evidence that the interaction with negative polyelectrolytes significantly improves the stability of the dispersion of the HN suspensions, in a concentration-dependent manner. For NaPa, no intimate interactions are present and no difference is observed at increasing chain length. The stabilization of the HN/NaPA complexes is mainly connected with effect of pH changes due to polyelectrolyte hydrolysis. On the contrary, in the case of DNA, a significant interaction has found with different details dependent on the different single- or double-stranded DNA conformation.

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CO43 Molecular simulation of generalized Gaussian-core model

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Soft colloidal systems, such as core-shell particles and spherical polymer brushes grafted onto fine particles, often show characteristic structural formation. In this study, molecular simulations on generalized Gaussian-core model which describes the effective interaction between soft colloidal particles have been performed, and the phase diagram has been clarified in a three-dimensional system as well as in a quasi-two-dimensional system under geometrical confinement [1]. Dynamics in a striped liquid phase, which obeys layer structure with no long-range order, have also been numerically investigated. A novel numerical method, which is suitable for the study of such soft colloidal systems, has been also proposed and demonstrated their efficiency [1,2]. The physical properties of anisotropic spherical polyelectrolyte brushes have also been discussed.

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CO44 Site-specific attraction of surface colloids driven by gradients of liquid crystalline distortions

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The site-specific migration dynamics of small particles at the air-nematic liquid crystal (LC) interface is investigated, using a LC film with a unique gradient of LC distortions. As the result of comparison between the dynamics obtained by experiments and theoretical model, the introduced gradient has been identified as the direct origin of the site-specific migration, while the elastic multipole interaction between the pre-existing distortion and that induced around particles is negligible. The results reveal a basic behavior of small particles with weak anchoring strength in LC distortions, which is often hidden in prominent elastic multipole interactions typically found with larger particles. Moreover, the present mechanism of the site-specific attraction of particles is specifically relevant to directed patterning and manipulations of nano-particles in nematic LCs with distortions.

Reference: Soft Matter 15, 923, 2019

CO45 Non-Exponential Double-Layer Forces

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Forces between surfaces determine the phase behaviour of colloidal systems. Textbook examples of such forces are exponential double-layer forces between charged particles. These exponential forces are observed in monovalent salt solutions and multivalent salt solutions, where the charge of the multivalent ion is the opposite to the charge of the surface – multivalent counterion. If one switches the charge of multivalent ion and the signs of the ion and the surface charge are the same – multivalent coion, a surprising effect is revealed. Contrary to the intuition, the double-layer interactions are not exponential any more. The force profiles exhibit a sigmoidal shape, and are algebraic at low separation distances, while becoming exponential only at large distances. Here, we present measurements of these non-exponential forces between silica particles across aqueous solutions containing multivalent coions. Measurements are done with colloidal probe technique based on atomic force microscopy. Since silica surfaces are negatively charged, we use solutions of 1:z electrolytes, were z is the valence of the anion. The concentration and valence of these electrolytes are systematically varied to study the effect of salt on the shape and magnitude of the force profiles. The non-exponential behaviour is caused by the expulsion of the multivalent coions from the slit between the two surfaces [1]. Similar non-exponential double-layer interactions are observed in the presence of like-charged polyelectrolytes [2].

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CO46 Quantification of the structure of colloidal gas?liquid interfaces

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We have quantified experimentally the width and structure of the colloidal gas?liquid interface. Our model system comprises spherical colloids that are sterically stabilized in an apolar solvent. Colloidal gas?liquid phase-separation is induced through the depletion interaction, i.e., by addition of non-adsorbing polymer. The broadness of the resulting colloidal gas?liquid interface was probed using synchrotron X-ray reflectivity measurements at various points in the phase diagram. We find that the interfacial width is comparable to the size of the colloidal particles and that it scales in a mean-field fashion with the density difference. Our results further suggest that the density profiles are monotonic. The experimental results show excellent agreement with theoretical predictions based on free-volume theory and highlight that X-ray reflectivity experiments can be used to shed light on the intricate structure of these colloidal interfaces.

CO47 2D colloids in rotating electric fields: Tunable interactions and particle-resolved studies of generic phenomena

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Tunable interactions in colloidal suspensions attract great interest because of their fundamental and practical significance. Self-assembly process in suspensions of micro- and nanoparticles is a common phenomenon in nature, and it can be used to create new materials in photonics and catalysis. Apart from practical interest, colloidal systems are of great importance for fundamental studies, since they mimic molecular behavior and can be used in particle-resolved studies of generic phenomena in condensed matter.

In this work, we present our results of theoretical and experimental studies of two-dimensional colloidal systems wherein attractive interparticle interactions are induced and controlled by external rotating electric fields [1-2]. By placing two-dimensional colloidal systems in external electric field rapidly rotating in the plane of system, we can effectively induce interparticle attraction, which is long-range, tunable, and non-pair. Magnitude of the interaction is controlled by electric field, evolution of the system can be visualized using video-microscopy, that opens a way for particle-resolved studies of such fundamental phenomena as self-assembly, condensation and evaporation, melting and crystallization, spinodal decomposition, dislocation dynamics, nucleation and coalescence, surface phenomena etc. In the framework of presentation, we consider (i) novel experimental technology for particle-resolved studies of colloidal suspensions in rotating electric field [1]; (ii) optimal experimental regimes; (iii) results of pair interaction analysis [3]; (iv) a novel method for experimental data post-processing [2]; (v) phase diagram of a monodisperse system in external fields [4].

These results open novel prospects in fundamental and applied studies of many-body systems with tunable interactions, and, therefore, will be of interest to wide range of scientists in the fields of soft matter, physical chemistry, chemical physics, photonics, and materials science. Project is supported by RSF Grant no. 17-19-01691.

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CO48 Establishing uniform emulsions as a model system for studying dynamics and rheology across the glass and jamming transitions

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We study experimentally the microscopic dynamics in glass-forming emulsion systems, composed of micron sized oil droplets dispersed in a polar solvent medium. Microscopy and dynamic light scattering experiments reveal the slowing down of droplet diffusion and the heterogeneous dynamics in the glass [1,2]. We apply a well-defined constant force with a laser line trap on individual colloidal polystyrene probe particles seeded in a refractive index and buoyancy matched emulsion to study the driven or 'active' motion in fluid and glass states. Our experiments reveal intermittent dynamics around a de-pinning transition at a threshold force [3]. To probe the motion in jammed emulsions at higher densities we use diffusing wave spectroscopy (DWS), a dynamic light scattering technique developed for white, highly scattering soft materials. Using an improved DWS analysis approach, taking into account collective scattering contributions, we accurately measure the bounded translational motion of crowded oil droplets. The results we obtain for the elastic shear moduli, based on a generalised Stokes-Einstein relation (GSER), match very closely with mechanical measurements and model predictions as the droplets become more tightly jammed [4,5].

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CO49 A Method for Reversible Control over Nano-Roughness of Colloidal Particles

Beybin Ilhan (University of Twente and MESA+ Institute for Nanotechnology); C. Annink, D.V. Nguyen, F. Mugele, I. Siretanu, M.H.G. Duits

Colloidal particles often display a surface topography that is smooth down to the nanometer scale. Introducing roughness at this length scale can drastically change the colloidal interactions, adsorption at interfaces and bulk flow behavior. We report on a novel, simple method to induce and control nano-scale roughness on (water based) polymer latex colloids. Reducing the amount of dissolved gases in the aqueous phase from the electrolyte solution surrounding the particles, generates self-structured surface asperities with an amplitude that can be tuned via temperature and repetition of the treatment. Due to the viscoelastic nature of the polymeric asperities, a mild thermal treatment below the glass transition temperature can be used for nanostructure relaxation, so that the particles can recover to their original topography, making this method fully reversible. Roughness can thus be controlled without affecting the chemical composition of the colloidal surface. Experiments for varying particle size, polymer type and surface chemistry suggest a broad applicability of our method.

CO50 Single channel ionic transport in an etched boron nitride crystal

EMMERICH, Théo (ENS Paris); MOUTERDE,Timothe (ENS Paris) ; KALANGI, Vasu (ENS Paris) ; NIGUES, Antoine (ENS Paris) ; SIRIA, Alessandro (ENS Paris) ; BOCQUET, Lydric (ENS Paris)

Confining liquids at the nanoscale revealed rich novel fluid transport phenomena, with potential applications in ultrafiltration, desalinisation, and energy conversion [1, 2, 3]. To pursue this exploration, we design a new class of single-channel nanofluidic system. It consists in an assembly of two hexagonal boron nitride 2D crystals stacked on top of a pierced silicon nitride membrane. The channel is patterned in the bottom crystal using conventional SEM using the Electron Beam Induced Etching technique (EBIE) under water vapor atmosphere [4]. We report the system ionic conductance variation with potassium chloride concentration. The scaling behaviour indicates surface driven transport at law salt concentration which differs from measurements inside BN nanotubes[5]. This difference possibly arises from curvature effects.

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CO51 Dynamic properties and relaxation times of a cluster interacting superparamagnetic particles in an oscillating magnetic field

Zverev, Vladimir (Ural Federal University); Ambarov, Alexander (Ural Federal University); Elfimova, Ekaterina (Ural Federal University)

The study of the suspensions consisting magnetic particles that have unusual properties is one of the areas of research for soft magnetic materials including magnetorheological fluids. The report is devoted to a special type of particles used in the synthesis of modern ferrofluids, namely multicore particles. Multicore particles contain an ensemble of magnetic nanocrystals with different packing densities and their spatial structure is fixed by a polymer shell. In this work we investigate the dynamic response of a single cluster of an ensemble of interacting ferroparticles that are formed multicore magnetic particle. It is assumed that the relaxation of the magnetic moments occurs due to Neel mechanism. The dynamic response of a cluster of single-domain interacting particles are determined from the solution of the Fokker-Planck equation. The modified mean-field approach of first-order is used to take into account the dipole-dipole interaction. The time dependence of the magnetization is calculated to determine the effective magnetic moment and relaxation time. Two cases of the mutual orientation of the external magnetic field and the easy magnetization axis are considered and analytical dependences are obtained.

CO52 Fabrication of 2D Charged Colloidal Crystals by Electrostatic Particles Adsorption on Oppositely Charged Substrates

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Charged colloids are stabilized against aggregation because of the electrostatic interaction between the particles. When the interaction is sufficiently strong, the particles are regularly arranged to form ‘colloidal crystal’ structures. The major governing parameters of the interaction, which is a driving force of the crystallization, are particle volume fraction ϕ, the charge number of the particle Z, and salt concentration C_s. The crystals could be obtained for quite dilute colloids ($\phi \sim 0.01$), resulting in crystals having large particle separations. We have thus far investigated controlled crystallization of silica particles, whose Z values were tunable by varying pH of the dispersion medium. In our laboratory, unidirectional crystallization of silica particles has been examined by using gradients of pH and C_s [1], which enabled fabrication of centimeter-sized large colloidal crystals under appropriate conditions.

On the basis of these previous findings, here we examined fabrication of two dimensional (2D) charged colloidal crystals on substrates. We utilized electrostatic adsorption of 3D charged colloidal crystals on the oppositely charged glass surfaces. Van der Waals force was also a driving force of the adsorption. The positively charged glass surfaces were prepared by modifying with a silane coupling reagent, 3-aminopopyltriethoxysilane. A single layer of 3D colloidal crystals of negatively charged silica particles (diameter = 550 nm) could be adsorbed onto the glass surfaces, at sufficiently low salt concentrations. We could adsorb colloidal crystals having various values of particle volume fraction ($\phi = 0.01$ to 0.1). The arrangements of the adsorbed particles were studied by radial distribution function, obtained from microscope images of the adsorbed particles. The resulted 2D crystals were polycrystals, having a crystal grain size of approximately 50 μm.

Furthermore, by combining the unidirectional crystallization technique and the 2D adsorption, we could fabricate centimeter-sized 2D charged colloidal crystals adsorbed on the glass surfaces. Here we used diffusion-crystallization of silica colloids (diameter = 550 nm, $\phi \sim 0.15$) by diffusion of base. The resulted crystals were adsorbed to the glass surface to form 2D crystals. The radial distribution function taken at various locations showed that the adsorbed 2D crystals thus obtained had good uniformity.

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IN1 Kirigami fog nets

BINTEIN, Pierre (trioS.lab, Universit Libre de Bruxelles); CORNU, Axel (trioS.lab, Université Libre de Bruxelles); VANDEWALLE, Nicolas (GRASP, University of Liege); TERWAGNE, Denis (trioS.lab, Université Libre de Bruxelles)

In several arid coastal regions, fog is harvested by nets placed in dominant winds to catch water droplets. We study experimentally how flexible meshes deform with wind variations, avoiding clogging by capillary effects and maintaining a high fog collection efficiency. By considering aerodynamic, capture and drainage requirements together with mechanical constraints, we propose an optimal geometry for kirigami nets.

IN2 Equilibrium phases of soft macromolecular confinement

BISWAS, Subhadip (University of Sheffield); CHAKRABARTI, Buddhapriya (University of Sheffield)

In living cells, membrane nanotubes, also called tethers, play a major role in the intercellular transport. Such nanotubes serve as conduits for cellular proteins, DNA and other macromolecules to pass between cells. Thus it is really important to understand the effects of confinement of a polymer chain inside lipid tubule to get an understanding of its equilibrium thermodynamic and transport properties. Giant unilamellar vesicles (GUVs) serve as an experimental system in which statistical mechanical theories of soft macromolecular confinement can be tested.

Polymer confinement in a rigid geometry have been well studied[1], and the chain conformational properties have been well established via simulations, experiments, that agree with scaling calculations. Relatively less is known about conformational properties of a polymer inside a soft tube. A recent experiment has revealed that under soft confinement DNA can undergo a conformational transition from a swollen to a more compact phase[2]. A scaling theory[3] developed in this context predicts three possible phases of a polymer under soft confinement depending on the surface tension σ, the bending modulus κ of the membrane, and degree of polymerization N of the polymer. Motivated by these results we study the properties of flexible and semiflexible polymer chains confined in a soft lipid bilayer tubule via coarse-grained molecular dynamics simulations[4].

We find that the entropic pressure for flexible chains having their end to end distance greater than the equilibrium tubule diameter causes the tubule to deform[5]. However, the constant area constraint of Helfrich free energy imposed by the surface tension causes the tube radius to shrink to a value smaller than the equilibrium radius without the chain. This has important consequences on the scaling results and the ansatz used for a variational calculation to determine membrane shape. We obtain the equilibrium shapes and an analysis of fluctuations of the tubule chain system via coarse-grained molecular dynamics simulations and semi-analytical treatment[6].

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IN3 How Graphene and Hexagonal Boron Nitride get electrified in water?

BOCQUET, Marie-Laure (CNRS and ENS Paris)

The recent emergence of nanofluidics has highlighted the exceptional properties of graphene and its boron-nitride counterpart as confining materials for water and ion transport [1-4]. Surprisingly ionic transport experiments have unveiled a considerable electrification of the water-BN surfaces, with a contrasting response for its water-carbon homologue [1]. This surface charging was conjectured to originate in the differential hydroxide adsorption at the surface of these twin materials, but the considerable challenge of simulating the elusive hydroxide ion has precluded a proper explanation up to now. In this talk, we report free energy calculations based on ab initio molecular dynamics simulations of hydroxide OH- ions in water near graphene and hexagonal boron nitride (h-BN) layers. Our results disclose that both surfaces get charged through hydroxide adsorption, but via strongly different mechanisms. The hydroxide species shows strong chemisorption on the h-BN surface, but only weak physisorption on the graphene surface [5]. Interestingly OH- is accordingly shown to keep a very fast lateral dynamics and interfacial mobility in the physisorbed layer on graphene. This behavior sheds new lights on the experimental results on ionic transport in carbon channels. Taking into account the resulting large ionic surface conductivity, an analytical transport model allows to reproduce quantitatively the experimental data [5]. Our results offer new foundations for the chemical reactivity of carbon and BN materials in water and suggest new perspectives in the context of advanced membrane technologies for water purification and energy harvesting [6].

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IN4 Nanotribology of ice

CANALE, Luca (Ecole normale supérieure de Paris); COMTET, Jean (Ecole polytechnique fdrale de Lausanne); NIGUES, Antoine (Ecole normale supérieure de Paris); SIRIA, Alessandro (Ecole normale supérieure de Paris), BOCQUET, Lydéric (Ecole normale supérieure de Paris)

The slipperiness of ice is an everyday-life phenomenon which, surprisingly, remains controversial despite a long scientific history. The very small friction measured on ice is classically attributed to the presence of a thin self-lubricating film of melt-water between the slider and the ice. But while the macroscale friction behavior of ice and snow has been widely investigated, very little is known about the interfacial water film and its mechanical properties. In this study, we develop a new force measurement technique based on a macroscopic tuning fork, to uncover the microscopic mechanisms underlying ice lubrication. A glass bead is glued on its prong and the tuning fork is excited at its resonant frequencies to induce both a lateral and perpendicular movement of the bead. When the bead is brought in contact with an ice surface, for the very first time, we simultaneously measure the induced shear-friction and quantify the in-situ mechanical properties of the interface as well as its thickness, under various regimes of speed and temperature. Our experiments show an unexpected mechanical behaviour of the interfacial film, which exhibits the visco-elastic response of a complex fluid, casting a new light on ice slipperiness.

IN5 Electrical Double Layers Close to Ionic Liquid-Solvent Demixing

CRUZ, Carolina (Institute of Physical Chemistry of Polish Academy of Sciences); CIACH, Alina (Institute of Physical Chemistry PAS); LOMBA,Enrique (Rocasolano Institute of Physical Chemistry); KONDRAT, Svyatoslav (Institute of Physical Chemistry PAS)

Electrical double layers (EDLs) play a key role in energy storage and have been suggested to have applications in energy generation. Recently, there has been an expansion of interest in EDLs, but EDLs with ionic liquid?solvent mixtures (ILSMs) received less attention. Herein, we study the temperature dependence of EDLs with ILSMs, in particular, close to demixing. We demonstrate the emergence of a bird-shaped capacitance, in addition to the well-known camel and bell shapes, which manifests the fine interplay between the electrostatic and wetting properties of ILSMs. We find that the capacitance increases appreciably as the system approaches demixing and this increase is accompanied by a sizeable enhancement of the energy storage.

IN6 Effect of nano-confinement in the phase behaviour of hard platelets

DIAZ-DE ARMAS, Ariel (Universidad Carlos III de Madrid); MARTINEZ-RATON, Yuri (Universidad Carlos III de Madrid); VELASCO, Enrique (Universidad Autónoma de Madrid); GURIN, Peter (University of Pannonia); VARGA, Szabolcs (University of Pannonia)

The effects of slit confinement on the phase transitions of liquid crystals has been an active line of research in the last decades. While most efforts have been directed to the study of capillary nematization/smectization of confined hard rods, platelets have received less attention. In this work we study the effect of nano-confinement on the phase transitions of a fluid of hard platelets of aspect ratios equal to 3, 6 and 9. The pore width is selected in such a way that only one particle fits into the slit when its axis is oriented parallel to the wall. We have found interesting phase behaviour:

(i) The presence of layering transitions between smectic phases with different number of layers, formed by platelets with axes perpendicular to the layers (planar configuration).

(ii) Phase transitions between two smectic phases with planar and homeotropic orientations occurring for very narrow pores.

(iii) The homeotropic smectic can further exhibit a second order transition to a biaxial smectic phase at high chemical potentials.

We calculated the phase diagram in the chemical potential-pore width plane by using the fundamental measure density functional for a fluid of hard board-like particles in the restricted orientations (Zwanzig) approximation.

IN7 Interface properties of phase separated colloid-polymer mixtures

DOHNI, Balkis (University of Oxford); ABDUL RAZAK, Huzaifah (University of Oxford); VERHOEFF, Lia (University of Oxford); AARTS Dirk G.A.L. (University of Oxford); DULLENS Roel P. A. (University of Oxford)

Liquid-liquid interfaces in phase separated colloidal suspensions have an ultralow interfacial tension. We study aqueous colloid-polymer (PMMA-Xanthan) mixtures, where the presence of non-absorbing polymers induces an attraction between the colloidal particles via the depletion interaction. This leads to phase separation in a colloid-poor (polymer-rich) ‘gas’ phase and a colloid-rich (polymer-poor) ‘liquid’ phase.

In this system, thermal capillary waves at the interface can be directly visualised and studied with confocal scanning laser microscopy. We analyse the capillary fluctuations of the interface between the two phases, which gives access to interfacial properties such as the surface tension, capillary length and time. In addition, we use optical tweezers to actively manipulate the interface between the liquid and the gas phase. This allows the study of the deformation and relaxation of the interface which shows different behaviours whether we use low laser power or high laser power, where we trap a whole drop of liquid.

IN8 Small molecule segregation in poly(vinyl alcohol) films

FONG, Rebecca (Durham University); THOMPSON, Richard (Durham University); COURCHAY, Florence (Procter & Gamble)

Molecular migration concerns a huge number of industrial systems containing mobile components in polymer matrices. The behaviour of surfactants at polymer interfaces is relevant to a wide range of systems in which polymer films encounter surfactant-rich environments, but predicting the behaviour of surfactants in polymer films remains a fundamental challenge. In this work, attempts are made to isolate parameters responsible for the blooming of surfactants and plasticisers from poly(vinyl alcohol) in order to predict and control segregation.

The segregation of surfactants and plasticisers from PVA films has been explored using neutron reflectivity to depth profile film components. A rich and diverse range of behaviours has been identified, which is affected by the nature of the surfactant and any additional plasticisers. For example, when PVA contains the anionic surfactant sodium dodecyl sulfate, a wetting layer of surfactant on the film surface is formed. In the presence of an additional plasticiser (glycerol) this SDS surface excess is greatly enhanced, and smectic nanostructures are formed, consisting of surfactant lamellae separated by interstitial glycerol layers.[1] Exploring the effect of film thickness on the surface nanostructure reveals that the number of surfactant lamellae increase with film thickness, strongly indicating the thermodynamic nature of this effect. The segregation behaviour of non-ionic and cationic surfactants from PVA contrasts this, with a much lower degree of segregation and influence of plasticiser observed.

Efforts are made to understand the driving forces behind these contrasting behaviours, to enable segregation to be ultimately predicted and controlled. Studying the film components in aqueous solution can provide insight into the role of surface energy in their migration and segregation. It was found that although surface energy arguments can be used to rationalise segregation to some extent, they cannot alone explain the plasticiser enhancement of the surface excess of SDS or the limited segregation of cationics.

We therefore additionally turn to the compatibility of film components, assessing this as a likely driving force for segregation. Determining the phase behaviour of model systems has proven to be a valuable tool for rationalising and predicting segregation.

Finally, positron annihilation lifetime spectroscopy has been used to better understand the free volume properties of the polymer in the presence of different plasticising molecules. This can provide insights into how the properties of the polymer matrix can influence migration and segregation of small molecules.[2]

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IN9 Tailored bicontinuous soft solids for energy applications

FRENCH, David (University of Edinburgh); MARENDUZZO, Davide (University of Edinburgh); MUNTZ, Iain (University of Edinburgh); THIJSSEN, Job (University of Edinburgh)

We present the first examples of bicontinuous interfacially jammed emulsion gels ('bijels') with a designed gradient in the pore size along the sample. These samples are created by quenching binary fluids which have a gradient in particle concentration along the sample, since the pore size is determined by the local particle concentration. We achieve the gradient in local particle concentration by loading the sample in two separate stages, using different particle volume fractions in each stage. We compare our experimental results to simulations, and use confocal microscopy to measure the pore size of the samples, finding gradients in pore size of approximately 2 microns per millimetre.

Such tailored soft materials could be optimised for both high ionic transport rates and high interfacial area, making them potentially useful in novel energy applications where both high power and high energy density are desirable.

IN10 Model Complex Fluids with Dispersed Clay Particles

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Clay particles can be used as quite planar hydrophilic surfaces to that we expose a bicontinuous microemulsion. As shown in grazing incidence and bulk small angle neutron scattering experiments lamellar order is formed adjacent to the interface. The dynamics of this interphase is faster and gives rise to the lubrication effect. This in turn could also be monitored by macroscopic rheology measurements, where larger clay particles give rise to better ordered lamellae that allow for a facilitated flow. For some crude oils as complex fluids as such, the viscosity could be even reduced. Apart from the more diluted studies up to 1%vol clay, we extended the concentration range to nearly 3% in order to follow the capillary condensation. When the mean distance of the particles is narrowed, the lamellar interphase prevails at some point, and extends over the whole volume. In this context different contributions to the free energy are discussed to explain the experimental results.

IN11 Molecular migration in semi-crystalline polymer films

GIBSON, Colin (Durham University); THOMPSON, Richard (Durham University)

Amphiphilic molecules are frequently used as additives in many polyolefin blends. These amphiphiles have been observed to self-organise and migrate to the surface of polymers [1] during processing and after extrusion, affecting the performance and shelf life of these products. Amphiphilic additives perform two key tasks: they impart desirable surface properties such as enhanced wettability and improve the processing of the blend by affecting the amount of wall-slip that occurs during extrusion. These properties are highly important for the manufacture of babycare and feminine hygiene products where wettability is required. It is therefore of great interest to determine the influence of aging and storage conditions in order to determine how these affect the additive distribution. Furthermore, the intrinsic properties of the materials themselves may also have a significant impact on how the additives behave within a finished product.

We have investigated the compatibility of a semi-crystalline, non-polar polymer and a non-ionic amphiphile. This has shown that the two components are only compatible when very small quantities of the additive are used, meaning that the additive is more likely to migrate to the polymer-air interface. This has been confirmed by ion beam analysis and the thickness of the surface excess produced has been measured. Our work has also shown that this surface excess is sufficiently mobile that interface is able to evolve over time. Losses of amphiphile from the surface can be replaced from the bulk, showing the ability of the amphiphile to migrate to the interface in films. This loss of additive elucidates the processes during use: on contact with aqueous liquids, the additive is able to migrate into the water and more molecules can migrate from the bulk. This evolution has also been shown in surface morphology investigations, with a change in surface feature sizes being observed with varying temperatures. This temperature effect has substantial implications for the optimum storage conditions of the finished product as this change of additive distribution may impair the normal function of the product.

We have also produced depth profiles of samples above the melting point of the polymer. These profiles are then compared to depth profiles of samples below the melting point of the polymer in order to identify the effect of crystallinity on the migration of the additive.

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IN12 Membranes at the Solid-Liquid Interface Studied with Grazing Incidence Neutron Spin Echo Spectroscopy

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Neutron spin echo (NSE) spectroscopy has the highest energy resolution in neutron scattering. This is achieved by encoding the energy transfer during scattering in the degree of polarization of a polarized neutron beam. The length scales and time scales accessible by NSE spectroscopy match those of thermally activated fluctuations in soft matter systems, such as polymer chains in the melt, phospholipid bilayers or microemulsion membranes.

NSE has been recently applied also to surface studies at the solid liquid interface. One example is phospholipid membrane dynamics on a rigid substrate [1]. Measuring with a highly collimated beam in one direction, the dynamics at different penetration depth can be studied with Grazing Incidence NSE spectroscopy (GINSES), using the same sample geometry as in Grazing Incidence Small Angle Neutron Scattering (GISANS). We found in phospholipid bilayers partially elastic modes with long wavelength, which agreed well to the expectation of a theoretical model by Romanov et al. [2].

The huge intensity penalty of the GINSES setup led to the development of new neutron optical components such as a neutron prism for a homogenization of the penetration depth for different wavelengths and a neutron resonator which increases the evanescent neutron field at the surface [3], which helped largely in conducting these studies of soft matter dynamics at the rigid interface.

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IN13 Mesoscopic modeling of ink penetration into paper

HULIKAL CHAKRAPANI, Thejas (University of Twente); K DEN OTTER, Wouter (University of Twente); LUDING, Stefan (University of Twente)

We present mesoscopic simulations of interfacial-tension-driven flows of simple and binary-mixture fluids from a reservoir into nanochannels, using many-body dissipative particle dynamics (mDPD). For simple liquids the penetration depth into the nanochannel follows the Lucas-Washburn $\sqrt{t}$ law. Binary fluids, however, exhibit unexpected behavior with the lesser wetting fluid traveling further into the nanochannel. In addition, the penetration front is enriched in that fluid. This effect can be enhanced by increasing the wettability contrast between the two fluids and by reducing the radius of the nanochannel.

This problem falls under the broader scope of modeling ink penetration into paper, which is of relevance to the printing industry. Ink is comprised of binary mixtures and colorants, which are essentially colloids, among other constituents. Time permitting, we present results of penetration of colloidal suspensions into nanochannels.

IN14 Tailoring plasmonic response by Langmuir?Blodgett gold nanoparticle templating for the fabrication of SERS substrates

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The development of nanostructured materials based on the self-assembly of simple constituents mediated by soft matter methods has been demonstrated to be an efficient and scalable bottom-up strategy. In particular, nanoparticle self-assembly is a robust and versatile strategy for the development of functional nanostructured materials, offering low-cost and scalable methods that can be fine-tuned for many different specific applications. In this work, we demonstrate a pathway for the fabrication of tailorable quasi-two-dimensional colloidal lattices of gold nanoparticles to be used in Surface Enhanced Raman Scattering (SERS) detection of biomolecules. This is a powerful and sensitive detection technique but is hampered by the low reproducibility and low uniformity of substrates used so far.

In the experiments presented here, functionalized nanoparticles are spread as a monolayer at the water/air interface, compressed to a target lateral density, and transferred to a properly functionalized substrate surface using the Langmuir?Blodgett technique [1]. Once firmly adhered to the substrate, the lattice of nanoparticles can be directly used or be further processed using electroless gold deposition to let the nanoparticle grow thus tuning the plasmonic response and SERS enhancement. Compared to direct deposition or self-assembly methods, our protocol enables to obtain consistent results and much higher coverage of Au nanoparticles thanks to the active control of the surface pressure of the spread monolayer.

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IN15 Ordered nanostructure formation in fluid mixtures with antagonisic salts

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Adding just a small quantity of antagonistic salt to a fluid mixture close to the critical point of demixing can lead to the spontaneous formation of ordered lamellar nanostructures consisting of oppositely charged fluid microphases. Using a multicomponent lattice Boltzmann method coupled to a Nernst-Planck solver for the ion concentration field we were able to demonstrate how these nanostructures form nematically ordered domains which grow at a rate proportional to the salt concentration. Above a critical upper salt concentration the structures suddenly dissolve completely, both in experiment as well as in our simulations. By exploiting the strong coupling of charge and fluid composition to approximate the charge field as a polynomial function of the fluid order parameter we managed to explain this observation as the result of a vanishing surface tension due to electrostatic contributions. Curiously, the coupling of charge and fluid composition also allows the system to be well approximated by the simple Ohta-Kawasaki free energy model, commonly used to describe diblock copolymer mixtures. Indeed in simulations we also find other 3D structures predicted by the Ohta-Kawasaki model beyond the lamellar ones so far observed in experiment by varying the volume fractions of the constituent fluids. To conclude we will give a brief outlook on our most recent efforts to better capture the microscopic detail of the delicate nanostructures of almost monomolecular width formed by the antagonistic salt sodium tetraphenylborate in a mixture of 3-methylpyridine and heavy water via molecular dynamics simulations.

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IN16 Self-assembled Copolymer Adsorption Layer-Induced Block Copolymer Nanostructures in Thin Films

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Polymer thin films usually entail adsorption layers originated from irreversible adsorption of polymer chains on solid substrates, which layers govern the entire properties of films. Similarly, the adsorption layer exists in the microphase separated block copolymer (BCP) films, playing a critical role in their self-assembly. However, understanding on the adsorption layer in BCP films remains elusive, and thus its effective control is more challenging. Herein, we employ self-assembled copolymer adsorption layers (SCALs), transferred from the self-assembly of BCPs at the air/water interface, as an effective way to control adsorption layers in BCP thin films. SCALs are irreversibly adsorbed onto substrates and can replace the natural adsorption layer when other BCP is additionally coated. We further show that SCALs guide the thin film nanostructures as it provides topological restrictions and enthalpic/entropic preferences for BCP self-assembly. Thus various novel nanostructures of SCAL-induced self-assembly are introduced such as arrays of spacing-controlled hole/dot pattern, dotted-line pattern, dash-line pattern, anisotropic cluster pattern, and so on.

IN17 Geometry of the particle monolayer on Pickering emulsions droplets

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Colloidal particles confined to two-dimensional fluid-fluid interfaces display a rich phase behaviour; depending on density and interactions they form aggregates or repulsive lattices, as well displaying the isotropic, hexatic, and crystalline phase transitions peculiar to two-dimensional fluids. Among other applications, the arrangement of particles at interfaces is of practical importance in particle-stabilized emulsions, or Pickering emulsions. As on flat interfaces, a range of morphologies has been observed on the surfaces of spherical fluid droplets, from aggregates to hexatic or crystalline packings. While hexatic order on spherical interfaces has been well studied experimentally via carefully tuned crystalline arrangements of repulsive particles on droplets, we here investigate the degree to which hexatic order or isotropic packing prevails on the densely coated surface of a Pickering emulsions resembling those found in industrial contexts. To this end, a surfactant-free water-in-oil model emulsion coated with sterically stabilized PMMA microparticles is produced. The micron-scale particles are individually resolved and tracked via confocal fluorescence microscopy, allowing for a precise characterization of order within the interfacial particle layer. Because the system exhibits a dense monolayer of particles, it represents a stable emulsion for practical applications but also resembles an experimental realization of a two-dimensional hard-disk fluid on a sphere.

IN18 Oscillatory depletion forces present between silica microparticles in solutions of various polyelectrolytes

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Various industrial applications including papermaking and water treatment require knowledge of the properties of particle suspensions, such as their stability and rheology. These parameters can be modified by the addition of polyelectrolytes.

The research was concentrated on the interaction forces between silica particles measured in aqueous solutions of poly(2-vinylpyridine) (P2VP), poly(L-lysine hydrobromide) and polyamidoamine (PAMAM) dendrimers using the colloidal probe technique based on an atomic force microscope (AFM). Observed forces were described by a superposition of damped oscillatory forces and double layer forces quantitatively. The double layer forces were modeled using Poisson?Boltzmann (PB) theory for a mixture of a monovalent symmetric electrolyte and a highly asymmetric electrolyte, whereby the multivalent coions represent the polyelectrolyte chains.

Results of the investigations show that the polyelectrolyte concentration change has an influence on the parameters characterizing oscillation forces. It was also proved that the increasing roughness of the silica particles deriving from the adsorbed cationic polyelectrolyte does not influence the presence of the oscillatory forces.

IN19 The Role of Chain Splay in Probing the Changes in Lipid Molecular Shapes at Variable Conditions.

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Owing to inherent amphiphilic properties, lipid molecules self-assemble into a remarkable range of structures when mixed with water. A vast majority of lipids form ‘inverse’ (type 2) whereas a few of them organize into ‘normal’ (type 1) self-assemblies, correspondingly, due to adoption of ‘inverse conical?’ and ‘conical’ shapes. Lipids formulate planar (lamellar) phases (type 0) when they acquire an average cylindrical shape. Israelachvili’s famous shape factor, also known as critical packing parameter (CPP) qualitatively describes lipid molecular shapes [1]; however, a well-defined method that can quantify molecular shapes remains elusive.

Recently, we reported a method to calculate an important parameter of amphiphilic molecules called ‘chain splay’ [2], and discussed its significance in understanding the relationship between molecular structure and pertinent molecular shape within self-assemblies. Here, we progress to the next level and present an applications of chain splay in probing the changes in molecular shapes at variable conditions of temperature, pressure and hydration. We also elucidate how lipid self-assemblies captivate these molecular level changes and tweak their lattice parameters.

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IN20 Soft Matter at a rubbing interface: a therapeutic application in total joint arthroplasty

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Wear debris from gliding interface of articular joint implants, such as bearings in total hip replacement (THR) and total knee replacement (TKR), has long been recognized as the principal cause of bone resorption after surgery. In response to particulate wear debris, a cascade of adverse immune responses is initiated, followed by osteolysis and loosening, which may lead to failure of the implants. Compared to the biological cure approach e.g. gene therapy to control the local inflammatory reaction, material science approach may provide a rather straightforward solution to this problem. In fact, the progress in the implant materials in the past half a century has been primarily focused on the development of bearing materials with improved wear-resistant properties. In this study, we propose a markedly different approach though; instead of material development and/or modification, we aim to suppress the wear of bearings by injectable fluidic lubricants to the joint implants. This approach is based upon recent progress in soft matter lubricant additives, e.g. brush-forming polymers, that improve anti-friction, anti-wear properties of various materials in aqueous solutions. The first target to test the feasibility of this approach is ultra-high molecular weight polyethylene (UHMWPE), a most commonly used bearing material as acetabular cup lining. Pin-on-disk tribometry and hip joint wear simulator (ISO 14242-1) were employed to assess the frictional and wear properties of UHMWPE, respectively, in serum as model synovial fluid, with or without fluidic lubricants. Fluidic lubricants were formulated by dissolving amphiphilic triblock copolymers, PEO-PPO-PEO (Pluronics, ?F127? for instance) in aqueous buffer solution (HEPES, 1 mM with no extra salts). The concentration of the amphiphilic copolymers was varied from 0.1 % (1 mg/ml) to 20 % (200 mg/ml) in HEPES buffer. For in-vitro cytotoxicity tests, cell morphology and MTT tests were performed by employing murine fibroblast (L929 fibroblasts) and murine osteoblast (MC3T3). Frictional tests showed that the fluidic lubricants display an immediate reduction in the coefficient friction upon injection into serum in which the sliding contacts between CoCrMo pin and UHMWPE disk are taking place. Wear tests of UHMWPE cup after 1 million cycles in hip joint wear simulator showed that gravimetric wear of UHMWPE in serum with F127 was reduced to the level of ca. 20% that in serum alone. Lastly, MTT tests showed that in-vitro cell viability of fibroblast and osteoblast exposed to F127 was comparable to a control when they were exposed to HEPES and cell culture medium only. The experimental results in this study collectively support that the proposed approach in this study, i.e. administration of fluidic lubricants for prosthetic joints, has a high potential to be effective in reducing friction and wear, and thus ultimately improving the longevity of the joint replacement implants. Further details on the lubrication mechanism of polymers at the rubbing interface will be discussed.

IN21 Migration of amphiphilic molecules in a curable polymer matrix

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We investigated the migration of small molecules through a curable polymer matrix. This migration is a key process in the functioning of a modern class of marine antifouling coatings: fouling-release coatings. The resulting enrichment of surfactant molecules at the polymer-water interface lowers the strength of adhesion between the foulant and substrate, allowing the removal of fouling species through hydraulic action. Improving understanding of the molecular migration process, including the factors driving the migration, may allow for improved design and formulation of these coatings.

A model system was used consisting of the nonionic surfactant $C_{12}E_4$ dispersed in cross-linked PDMS. The distribution of the amphiphilic molecules were explored using Water Contact Angle Analysis, Atomic Force Microscopy, and Nuclear Reaction Analysis. In addition, factors affecting the distribution and also diffusion of the surfactant were explored.

During immersion in water, the surfaces underwent a change from hydrophobic to hydrophilic, demonstrating that exposure to water stimulates the migration of surfactant from the PDMS bulk to the water/PDMS interface. The surfactant was observed to have a homogeneous distribution throughout PDMS films in air, with a possible surface depletion at 8% $C_{12}E_4$, providing an explanation for the initial hydrophobicity of the films. The observed migration is likely the result of a reduction in the surface energy, with the air/PDMS surface free energy being less than that of air/$C_{12}E_4$, but the water/PDMS interfacial energy being greater than that of water/$C_{12}E_4$. As such, a key driving force for the molecular migration in this system has been identified to be the surface free energy.

IN22 Electro-hydrodynamic coupling in ionic transport through one-nanometer radius carbon nanotubes

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Nanoscale confinement of fluids and ions revealed numerous exotic transport properties [1], such as enhanced permeability in carbon nanotubes [2] or reduced ion mobility in ngstrm-size slits [3]. In this work we report first measurements of the pressure-induced ionic current (streaming current) through single one-nanometer radius carbon nanotubes.

These measurements revealed a large electroosmotic mobility compared with the one reported for boron nitride nanotubes [4]. This mobility translated in terms of zeta potential is on the order of several volts. This high value is believed to be related to the large slippage expected in small carbon nanotubes [2]. Furthermore, we observed that the streaming mobility is linearly controlled by the applied bias voltage, reminiscent of the voltage-gated streaming response recently reported [5]. Finally, above a critical pressure gradient the streaming current varies strongly non-linearly with pressure. This behavior is also observed to be pH-dependent.

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IN23 Utilising Force Spectroscopy to Investigate Desorption and Single Chain Pull-out from Polymer Thin Films

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The fundamental behaviour of polymers at interfaces is governed by intermolecular and surface forces at the single chain level. Understanding and characterising these forces is vitally important for many applications, such as composite materials and the miniaturisation of devices and sensors. We hereby present an AFM force spectroscopy study which characterises the fundamental interactions between single poly(styrene-co-butadiene) (SBR) random copolymer chains and mica, silicon, and graphite substrates at the nanoscale. Furthermore, the forces associated with polymer desorption from the silicon AFM tip and extracting polymer chains from a thin film were also identified.

Thin films of SBR were prepared on each substrate using dip coating, and AFM force spectroscopy with a silicon tip was utilised to measure the forces associated with desorbing the chains from the substrates/thin films. The results demonstrated that the interactions were the strongest between the SBR chains and the graphite substrate. This is in agreement with our previous AFM imaging observations where the SBR formed nanostructures with low contact angles and large surface coverages on the graphite surface, such as continuous networks and nanoribbons. Furthermore, aromatic stacking is speculated between the styrene units in the SBR chains and the graphite surface. The magnitude of the polymer desorption force was very similar on the silicon substrate and the silicon AFM tip, which was expected, as both are composed of similar materials. The desorption force on the silicon substrate/tip was smaller than on the graphite substrate. The interactions between the SBR and mica were the weakest of the three substrates. This is also in line with our AFM imaging observations where the SBR minimised surface contact with mica and formed spherical cap shaped nanodroplets with fairly large contact angles. In addition to agreeing with previous AFM imaging results, the measured desorption force values also correlate with theoretical calculations of interfacial adhesion for each system and the water contact angles of each substrate. The most common phenomena to occur during the experiments on each substrate was polymer/polymer interactions associated with chain pull-out from the thin films. However, the force of chain-pull out was weaker than any of the polymer/substrate interactions.

We have used an uncomplicated and highly efficient experimental system to characterise the intermolecular and surface forces which govern polymer behaviour at interfaces. Each phenomena that occurred during the experiments was quantified and the force associated with chain pull-out was investigated for the first time. These results are useful to fundamental polymer science, as well as, many applications such as polymer/carbon composite materials.

IN24 Out-of-equilibrium active membranes: incorporation of bacteriorhodopsin in a floating lipid bilayer

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Transmembrane proteins have a pivotal role in the large number of cellular processes and provide essential functions of the cell membranes. By itself, membranes exhibit thermal fluctuations, but membrane protein activity breaks the fluctuation-dissipation theorem leading to out-of-equilibrium fluctuations. Active fluctuations have been widely described theoretically [1], but there are only few techniques for their experimental study. The outstanding model system as fluid floating phospholipid bilayer [2] and original scattering techniques as off-specular reflectivity [3] gave us ability to study the fluctuations of a single floating bilayer near a substrate [4] as well as membrane-membrane interactions [5]. The main aim of this project is to investigate out-of-equilibrium fluctuations of phospholipid membranes induced by active transmembrane protein bacteriorhodopsins (BR). Model systems such as tethered phospholipid bilayer, solid-supported single and floating phospholipid bilayers, prepared by Langmuir-Blodgett/Langmuir-Schaefer techniques, are routinely used to mimic and study phospholipid membranes and their interactions. As a first step the detergent-mediated incorporation method [6] was adapted to perform the insertion of BR into the phospholipid bilayer at the interfaces, using such sugar-based detergents as DDM and DOTM. We present the proof of the possibility of inserting BR in supported POPC phospholipid bilayers and in a double bilayer system consisting of DSPC (bottom, supporting bilayer) and DPPC (top, floating bilayer) as recently demonstrated by neutron and x-ray reflectometry, QCM-D, fluorescence microscopy and AFM. Newly developed sample environment - solid-liquid cells suitable for the NR, XRR synchrotron and inhouse measurements, with the ability of sample illumination during measurements and solution injections – will be demonstrated. A further step of this work will be to check the protein activity, which can be triggered by the absorption of the green light, in the supported bilayer systems by means of NR. The lateral features of the membrane embedded proteins system and then out-of-equilibrium fluctuations caused by the protein activation will be probed by synchrotron radiation off-specular measurements.

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IN25 Interaction Between Nearly Hard Colloidal Spheres at an Oil-Water Interface

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We report measurements on the structure of, and interaction between sterically stabilised colloids at an oil-water interface. It was first reported in 2017 that poly(methyl methacrylate) particles exhibit a long range interaction at an oil-water interface [1], despite a hard sphere interaction being reported in the oil phase [2]. From experimentally measured radial distribution functions, g(r), we extract interparticle potentials using a reverse Monte Carlo scheme, minimising the difference between simulated g(r) and experimental g(r).

Using a blinking optical trap (BOT) setup, we also directly measure this interaction in both the bulk oil phase and at the interface. We find that, using the conventional poly(12-hydroxystaeric acid) (PHSA) steric stabiliser, the particles exhibit a long range repulsive interaction, contrary to previous reports. However, upon substituting PHSA for poly(lauryl methacrylate) (PLMA) a hard sphere potential is measured in the bulk, while a long range interaction does appear when the particles adsorb to the interface.

Fits of the measured interparticle pair potential, U(r), show a negligible dipole contribution, suggesting that previous models [3, 4] do not apply to this system. A Bayesian analysis on the BOT measurements indicates, for each U(r) curve, a model requiring only a screened monopole term, rather than a combination of this with a dipole term, is 5 times more likely to fit the data. Using the knowledge that water-alkane interfaces are charged [5], we postulate that this monopolar screened interaction arises mainly through the repulsion of neutral holes on a charged interface.

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IN26 A model of tethered lipid bilayers using anchor-harpoon surfactants on designed electrodes

Ophelie Squillace (Durham University)

Models for biological membranes are essential to address fundamental studies regarding membrane-membrane interaction, the functionality of proteins, the dynamics of ions through the membrane and its structure in itself. Maintaining the membrane hydrated, fluidic and close to the substrate without cumbersome chemistry can be a challenge. Here, we develop a new experimental approach where a single model phospholipid bilayer is kept fluid and partially tethered to a flat electrode. We proposed an original anchoring surface functionalization that is highly reactive to –OH terminated molecules. In this way we avoid complex organic chemistry and graft commercial Brij non-ionic surfactants chosen for: i) their appropriate hydrophilic chain length that forms an aqueous cushion for the membrane; ii) their hydrophobic alkyl block that anchors the lipid bilayers by insertion in their core. In this way, we keep the membrane fluidity in full immersion and presence of salts. This method appears to be a simple and cheap way to prepare tethered membranes with tunable anchoring densities on various supporting materials. Using transparent electrodes (ultra-flat and thin metal layers on glass), we could check the membrane fluidity and lipids dynamics from fluorescence techniques (such as in-situ FRAP for measuring the lateral diffusion of inserted fluorescent lipids). The transparent electrodes are also designed for high-resolution structure investigation of the single membrane using x-ray, neutron and light scattering methods (microscopies, Surface plasmon resonance, fluorescence). Tethering the bilayer on conducting substrates also open avenues for the use of cheap and easy to build membrane biochips for biotechnological applications.

IN27 Partitioning of flavors in polyvinyl acetate based matrices with polarity mismatch.

Ophelie Squillace (Durham University)

Poly(vinyl acetate) (PVAc) is a synthetic polymer whose possibilities of application and usage as a good alternative to non-biodegradable polymers can be extended to many industrial areas (water-dispersed resins food, packaging, adhesives?)1. In order to fulfil its desired role, such as the release of flavours, the final properties of the resin can be tuned by its formulation with small molecule plasticizers along with the degree of hydrolysis (DH) of PVAc. Despite a greater appreciation of the role played by molecular interactions, formulation design work is still largely based on trial and error rather than adequate understanding of polymer behaviour at the molecular level. Understanding how additives interact with resins and segregate to interfaces will help to reduce the over-engineering of these materials. Here, the experimental effort is part of a larger collaboration to study the migration of small molecules in complex polymer matrices, including lateral migration, analytical theory, and computational models. It provides invaluable data to test new computational and analytical models and attempts to identify the driving forces and factors that lead and influence additive segregation in diverse systems. The systems chosen for this study aim to address the effect of polarity mismatch, and then compatibility, between the migrants and the polymer matrix. As a non-polar resin polymer, PVAc is mixed with more polar migrants (sorbitol, octanoic acid (OA), and triacetin). Sorbitol and OA are both used in commercial formulations with PVAc, but have very different properties. Whilst they have comparable molecular weights, sorbitol is polar with six hydroxyl groups, whereas OA is relatively nonpolar with one hydroxyl groups. Atomic Force Microscopy (AFM), Contact Angle (CA) and thermal analysis have revealed that surface segregation of sorbitol occurs at low DH and is enhanced when compatibility decreases. Using ion beam analysis, it has been determined that OA is surface-active at high concentrations in PVAc and CA analysis on these films shows that the surface energy changes at concentrations as low as 5%w/w of OA. Adding triacetin, as a second migrant, has an impact on the segregation and is related to the shift of compatibility that the system undergoes. Compatibility is surely identified as one of the main driving force for the segregation in the systems studied. The solubility, polarity and functional groups of the additives also play an important role and competition can take place between surface tension and molecular weight of the migrants although compatibility still seems ahead to govern the migration of the components and organization of the matrix structure. As studies have been restricted to materials that are model-supported films under static conditions in a first step, it is also wished to address the more challenging conditions of materials under controlled stress or strain. To achieve this, a simple rig and PDMS cell has been designed to stretch the material and to probe these mechanical effects on the migration of additives AFM. This will make a significant step towards exploring the influence of extensional strain on surface segregation, flavour release, in cross-linked rubbers.

IN28 An effect of surface ordering on the smectic A to hexatic B phase transition in free standing smectic films

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The influence of the surface ordering and finite size on the phase transitions in liquid crystal (LC) films is considered. In LCs a free surface stabilizes a higher-ordered phase that is only observed at lower temperatures in the bulk or not observed in the bulk at all. This is in contrast to solids, which exhibit surface-induced disorder that can lead to surface melting. The results from the synchrotron studies of the free standing smectic films (FSSF) carried out in recent years are presented. The FSSF are particularly suitable to investigate the above problems: such films are substrate-free; the alignment of the smectic layers is almost perfect, allowing the study of single-domain samples of various thicknesses. Here we emphasize on the phase transitions in FSSF involving smectic A (Sm-A) and hexatic B (Hex-B) phases. These phases can be considered as a stack of parallel molecular layers, in which elongated molecules are oriented on average along the layer normals. The Hex-B is a three-dimensional (3D) analogue of a common hexatic phase predicted by Halperin and Nelson [1] for melting in 2D; it exhibits long-range bond-orientational order and short-range positional order within each layer. We present experimental and theoretical studies of a Sm-A to Hex-B transition in FSSFs of the 54COOBC compound [2]. Micro-focused X-ray diffraction in combination with Angular X-ray Cross-Correlation Analysis [3] revealed coexistence of the Sm-A and Hex-B phases at first order transition in these films. The temperature region of two-phase coexistence near the phase transition point diminishes with decreasing film thickness. The width of this temperature region as a function of the film thickness was derived on the basis of a Landau mean-field theory in the vicinity of a tricritical point (TCP). It is shown that close to TCP the surface Hex-B order penetrates anomalously deep into the film interior.

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IN29 Dynamic clustering regulates activity of mechanosensitive membrane channels

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Mechanosensitive protein channels regulate the flux of solutes between the cell and its environment in response to mechanical stimuli. Their activity is central to survival and adaptation of all organisms. Recent in vitro experiments have suggested that bacterial mechanosensitive channels separate into 2D liquid-like clusters, exhibiting non-linear gating activity. To understand the physical mechanism and functional role behind the process we develop a near-minimal coarse-grained model of mechanosensitive channels embedded in a lipid membrane, exposed to an osmotic shock. We characterise the gating activity of single and multi-channel systems, and find that the channel aggregation into liquid-like clusters promotes the closure of individual channels. The extent of clustering is highly dependent on the channel concentration and membrane stress. We show that such a system yields a tightly controlled gating activity, whereby at high tensions - immediately post hypoosmotic shock - channels gate individually, and at lower tensions the channels spontaneously aggregate into clusters and inactivate. We suggest that this positive feedback protects the cell against excessive loss of cytoplasmic content. Our results point to a novel role of functional micro-phase separation in the cell membrane, and outlay design rules for creating artificial nanomechanosensing systems.

IN30 Mechanical Characterization of Human Serum Albumin Microcapsules Using Electro-deformation Technique

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Understanding of the mechanical characterization of microcapsules is significant for their precise applications, such as in pharmaceuticals, cosmetics, agriculture, food industries etc. The implementation of the electrodeformation technique is known for the investigation of mechanical characteristics and kinetics of polysiloxane microcapsules. In the present work, we demonstrate the effect of microcapsule sizes and the concentration of human serum albumin (HSA) on the surface Young's modulus of the protein microcapsules using the electrodeformation technique. We observed that the surface Young's modulus increases with the sizes of the capsules as well as with the concentration of HSA which is in conjunction with the results procured by other techniques, such as, elongational flow as mention in the literature.

IN31 Effect of Adhesion on the shape transformation of vesicles.

RAVAL, Jeel (Institute of Physical Chemistry ,Polish Academy of Science); GÓŹDŹ, Wojciech (Institute of Physical Chemistry ,Polish Academy of Science)

We investigate shape transformations of lipid vesicles induced by their adsorption on a flat rigid surface. The calculations are performed within the framework of Helfrich's elastic energy, where the lipid bi-layer is modelled by a mathematical surface. The adsorption of vesicles with different reduced volumes and for different spontaneous curvatures of the bi-layer membrane has been studied. We probe the influence of the change in the adsorption potential on the shape and the energy of the adsorbed vesicles. Possible transitions between different classes of vesicles are examined.

IN32 Stimuli-Responsive Lipogel Capsules

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Previous work into lipid bilayers coupled to flexible substrates has shown that they can form reversible pores, whose diameter can be controlled by the magnitude of the substrate stretch (1). The aim of this work is to utilise the process of controlled pore formation in the design of stimuli-responsive lipogel capsules capable of releasing actives in response to external triggers.

We use inverse emulsion templating microfluidics to prepare polymer microgel beads stabilised by a lipid monolayer. The lipid bilayer membrane is then assembled using emulsion phase transfer.

Our next step is to create microgel cores which, by deforming upon external triggers (e.g. temperature, pH), will trigger the formation of pores in the membrane coating and the release of encapsulated actives for the duration of the stimulus.

(1) Sticking and sliding of lipid bilayers on deformable substrates, Stubbington L, Arroyo M, Staykova M, Soft Matter, vol. 13, issue 1 (2017) pp. 181-186

IN33 Dynamic boundary layers in charged nanopores

Rodrguez-Matus, Marcela (Université de Bordeaux); Zhang, Zaicheng (Université de Bordeaux); Maali, Abdelhamid (Université de Bordeaux); Wrger, Alois (Université de Bordeaux)

The transport properties of charged capillaries or nanopores depend to a large extent on the electric double layer. They are relevant for nanofluidic circuits and biotechnology applications such as DNA sequencing.

In many instances, the underlying electrokinetic effects are coupled to a non-uniform pressure, such as the fluxes of both volume and charge are driven by the electric field and the pressure gradient. The volume flow consists of Poiseuille and electro-osmotic contributions, and the charge current is determined by the electrical conductivity and advection of the diffuse layer by the Poiseuille flow.

Here we report on a recent experimental and theoretical study of the coupling of electric current and Poiseuille flow. Using dynamic AFM oscillating close to a solid wall, we have measured the force F on a sphere mounted on a cantilever. We find a linear dependence of the inverse damping coefficient in the sphere-wall distance h, as expected from lubrication theory. When comparing data for a 50 mM electrolyte solution with those for pure water, we observe a shift by about 100 nm, which indicates an effective channel width reduced by the screening length of the electric double layer.

In order to provide a clear physical picture, we have developed a theory for the viscous force in the presence of surface charges. The above equations for volume and charge flows are closed by Gauss? law and advection-diffusion equation for the ions. Thus we obtain measured enhancement of the viscous response. Our theory also provides the visco-elastic response, as a function of the product of the AFM driving frequency and the relaxation time of the non-equilibrium charge distribution due to advection. Finally, we give the oscillating charge induced by the confined film.

IN34 Designing responsive foams with an adjustable temperature threshold of destabilization

SAINT-JALMES, Arnaud (CNRS-Institut de Physique de Rennes); FAMEAU, Anne-Laure (INRA, Nantes); COUSIN Fabrice (LLB, CEA)

Responsive aqueous foams refer to foams for which the macroscopic stability can be switched between a stable and an unstable state [1]. The optimization of many processes such as washing or separation/recovery processes first require the formation of a stable foam, as well as the need to destabilize it in another step of the process. Our aim was to design thermoresponsive foams with a widely adjustable temperature threshold of destabilization.

We developed a green formulation: 12-hydroxystearic acid (12-HSA) mixed with counterions (alkanolamine) of different chain lengths, and at different molar ratio R between 12-HSA and the counterions [2-3]. First, by coupling microscopy techniques, DSC, SANS and X-ray scattering, we investigated the bulk structures, from the molecular to the mesoscopic scale. For all the counterions and depending on the temperature and R, either micron-size tubes or micelles were formed. We showed that tubes transitioned into micelles at a precise temperature. This temperature transition depended on both R and the alkyl chain length of the counterion and could be precisely tuned from 20C to 75C. We highlighted that the transition at the supramolecular scale came from the chain melting phenomenon at low R, and from the surface melting process of the hydrogen bonds at high R [2].

Secondly, at the macroscopic scale, we demonstrated that foams were ultrastable in the presence of tubes [3]. Moreover, by increasing the temperature above the tube-micelle transition temperature, the foams rapidly collapsed, precisely when tubes transform into micelles. Remarkably, by changing the counterion and R, the foam stability can be accurately tuned, with a transition temperature set to a value ranging from 20C to 75C (Figure 1). It is the first time that, by using a single surfactant, responsive foams are made with a temperature threshold varying over such a wide range of temperatures [3].

[1] S. Fujii, & Y. Nakamura. Langmuir, 2017, 30, 7365.

[2] A-L. Fameau, F. Cousin & A. Saint-Jalmes. Langmuir, 2017, 33, 12943.

[3] A-L. Fameau, F. Cousin, R. Derrien & A. Saint-Jalmes. Soft Matter, 2018, 14, 2578.

IN35 Miscible Two-fluid Channel Flow: Velocity Profiles and Hydrodynamic Stability

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Miscible fluids flowing side by side are frequently found both in natural and industrial environments. Although the fluid-fluid boundary eventually disappears upon reaching homogenization, it exists as a quite well-defined interface before the mixing occurs.

Despite its relevance for a wide variety of systems, from geosciences to fluid removal, the physics governing transient miscible interfaces is still scarcely understood, the main question being the existence of a transient interfacial tension and its role on mixing dynamics and flow stabilization.

By exploiting the microfluidic technology, we reproduced parallel flow situations in a controlled way and characterized their velocity profiles and investigated their hydrodynamic stability.

By comparison with immiscible systems, we found that, if the interface is not smeared out by diffusion, the velocity profiles show the same behaviour, while the stability properties are markedly different. Our experiments suggest that the surface tension plays a crucial role in the stabilization of two-fluid parallel flows: we have observed instabilities driven by flow rate differences only in systems of miscible liquids, mutually immiscible liquids being always stable. In this regard, the existence of a stability region even in the case of miscible liquids separated by a sharp interface could possibly contain information about some effective interfacial tension stabilizing miscible systems at low flow rate differences.

IN36 Sticky Slips

SHEK, Alvin (University of Durham); PANTER, Jack (University of Durham), SEMPREBON, Ciro (Northumbria University), KUSUMAATMAJA, Halim (University of Durham)

Inspired by pitcher plants, the so-called liquid infused surfaces are constructed by infusing rough or porous materials with a lubricant. They exhibit many advantageous surface properties, including self-cleaning, drag reduction, and anti-fouling. These applications exploit the fact that liquids move with very little resistance parallel to the surface. In contrast, here we will computationally study the displacement of liquids perpendicular to the substrate. Using Surface Evolver, we simulate the behaviour of a capillary bridge sandwiched between two LIS, and quantify the force. Interestingly, for LIS, we find the capillary forces are stronger when compared to the standard case of a capillary bridge between two smooth homogenous surfaces. We will also discuss the effects of varying the surface tensions of the fluid-interfaces and the size of the liquid bridge compared to the emerging lubricant ridge.

IN37 Controlled Interfacial Shear for Alignment of Cellulose Nanocrystals

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Developing sustainable replacements for current polymers is an ever-increasing field of interest, biopolymers provide a viable candidate for this. Cellulose is the most abundant biopolymer, already utilised in the pulp and paper industry in its fibrous form. When cellulose undergoes acid hydrolysis the loose fibril areas are removed leaving only rigid nanocrystals. These nanocrystals are of interest because they provide the backbone for building cellulose thin films with industrial applications such as lubricants. Previously, multi-layered systems of cellulose nanocrystals and hexagonal gibbsite platelets were constructed using the layer-by-layer approach.1 We aim to build on this work by exploring the chemistry-structure relationship of the layers, as well as functionalising these layers initially through flow alignment. Flow alignment cells are extremely important in interfacial surface chemistry and many industrial applications where liquid shear is important. Solid-liquid flow cells have allowed for the analysis of solid-liquid interfaces in neutron experiments, allowing the influence of shear flow across an interface to be observed in-situ. Current flow cells are only capable of flowing in one direction, however, to allow for more comprehensive alignment a two directional flow cell is needed.

The aim of this two directional flow cell would be for complete control over the alignment of soft matter self-assembled at surfaces as well as the possibility to functionalise these surfaces. Using computer aided design and 3D printing we have developed a novel solid-liquid flow cell which allows for flow in two directions, this flow cell will have a huge impact on the soft matter neutron community as it enables more even distribution of liquid in the solid-liquid cell and much improved alignment of the surface. This work has been undertaken in collaboration with CFD analysis of the flow cell designs, this has allowed for optimisation of the flow. The optimised design has been tested in neutron experiments, initially to observe whether there was any interaction between the neutrons and the resin chosen for printing. Secondly, the flow cell has been tested on the layer-by-layer built gibbsite/cellulose multilayer films, which has allowed for the continuation of previously conducted work on these systems. These new flow cell designs have enabled us to observe what structural changes happen to these systems under shear flow as well as opening the possibility for alignment and functionalisation of soft matter layers at interfaces.

1) C. Martin et al., Langmuir, 33(32) (2017) 7896-7907

IN38 Nanostructure of foamable polyol-rich CO_2-microemulsions

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In recent years the properties of microemulsions of the type water-scCO_2-nonionic surfactants, i.e. their phase behavior and nanostructure were systematically studied [1-2]. Besides fundamental questions, the Principle Of Supercritical Microemulsion Expansion (POSME) [3] which is a promising approach to produce low-cost, nanostructured polymer foams was the main driving force to study these new-type of microemulsions. State of the art polyurethane-foams exhibit a pore size of around 150-200 mikrometer and a thermal conductivity of 0.023 $Wm^{-1}K^{-1}$. The envisaged nano-foams are expected to have a thermal conductivity of only 0.015 $Wm^{-1}K^{-1}$, which makes them exceedingly attractive for thermal insulation applications. Within a research project we formulate foamable microemulsions of the type polyol-scCO_2-surfactant to use them as starting material for the POSME approach. By the addition of isocyanates, the mixture starts to polymerize while the mixture is expanded at the same time assuming that the nanostructure of the microemulsion is preserved. In this work, we first formulated and studied the phase behavior of foamable polyol-microemulsions as a function of temperature and pressure. In order to prove the existence of scCO_2 swollen micelles, SANS experiments were performed. Enhancing the scattering contrast using a partially deuterated polyol we found micelles in the binary polyol-surfactant system, which indeed could be swollen with scCO_2. We revealed that the radius of the CO_2 swollen micelles decreases with increasing pressure and decreasing temperature. Thus, these scCO_2-in-polyol microemulsions are very promising starting systems for the synthesis of PU-nanofoams.

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[3] R. Strey, T. Sottmann, and M. Schwan, Patent No. WO2004058386 (2003).

IN39 Ionic liquid phase transitions near charged, perfectly conducting electrodes

STENBERG, Samuel (Lund University); LU, Hongduo (Lund University); WOODWARD, Clifford (University of New South Wales); FORSMAN, Jan (Lund University)

We study structures, phase transitions and electrochemical behaviours of coarse-grained ionic liquid models near charged, perfectly conducting model electrodes. To this purpose we use Monte Carlo simulations and a recently developed classical Density Functional Theory (DFT), and in both methods we use uniformly charged electrodes while the polarization effects are modelled via screened image charges.

We use two different models to represent the ionic liquid, both derivatives of the Restricted Primitive Model (RPM). In these two models we represent the cations and the anions as hard spheres of equal size, with the difference that the cation is able to approach the surface more closely. The choice of models is based on the fact that the ionic liquid anions generally are spherical with a more or less central charge, while the cations are non spherical with displaced charges. The cations are thus favoured near a non-charged wall due to surface polarization.

Hence for a positively charged electrode, there is a competition at the interface between anions and cations, and for a range of positive voltages this generates a phase transition where the two phases are structurally quite different. This phase transition produces a dramatic drop in the differential capacitance.

DFT calculations predicts different surface charge densities at a given surface potential, indicating a phase transition. The DFT calculations motivated subsequent Grand Canonical Monte Carlo simulations which confirmed the behaviour. Using simulations, we were also able to monitor the spontaneous phase separation in terms of structural demixing at the interface.

IN40 Reactive foams: can we accelerate chemical reactions

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Liquid foams, which are composed of gas bubbles dispersed in a liquid phase, contain a large interfacial area and many liquid channels in which chemical reactions can be performed [1]. In this work we study the oxidation of metal copper, Cu, into Cu^{2+} ions in acidic conditions by O_2, taking advantage of the large quantity of O_2 contained in the foam bubbles. This reaction is of high interest in the field of hydrometallurgy for the recycling of the metals contained in IEEE wastes, which consists in oxidizing and dissolving metals in acidic solutions [2,3]. Using foams as a reactive media would enable to drastically reduce the volume of liquid effluents generated in these processes, which would enable to help the development of this recycling route.

Here we study the oxidation of a copper plate in a foam in which the continuous phase contains H^+ ions and the bubbles contain air. In this situation, the drainage flow controls the advection of the H^+ ions of the solution and of the dioxygen dissolved in the water while Oswald ripening controls the diffusive transport of O_2 from the bubbles to the Cu surface. We find that the oxidation of Cu in 100 mL of acidic foam leads to 4 times more Cu^{2+} ions than in 100 mL of solution, thanks to the fast diffusive transfer of O_2 through the thin films of the foam. Regarding the recycling of IEEE wastes, foams therefore combine two advantages: a faster chemical reaction and a strong reduction of effluents!

To study into more detail the coupling between the kinetics of the chemical reaction and the transport of the reactants through Oswald ripening and drainage flow, we develop an experimental set up where we impose a forced drainage flow of a hydrochloric solution through a foam containing a copper cylinder. We find that the diffusion of O_2 from the bubbles through the thin-liquid films of the foams is very fast and that the chemical reaction is limited by advection of the H^+ ions to the surface of Cu surface. By modeling this convection-diffusion-reaction problem we show how the structure of the foam can control the chemical reaction.

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IN41 Novel Amphiphilic Polycarbonate Di-Block Copolymers Applied to Nonionic Microemulsions

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Former studies revealed that, small amounts of amphiphilic poly(ethylene propylene)-block-poly(ethylene glycol) (mPEG-b-PEP) polymers are able to considerably increase the efficiency of medium-chain surfactants in forming microemulsions [1]. In this study, the influence of novel amphiphilic block copolymers which are of the type monomethoxy poly(ethylene glycol)-block-poly(butylene carbonate) (mPEG-b-PBC) on the properties of microemulsions are investigated. These degradable aliphatic polycarbonate di-block copolymers are synthesized via catalytic copolymerization of CO_2 and 1,2-butylene oxide (BO), starting from monomethoxy poly(ethylene glycol) (mPEG) as a chain transfer reagent. Since CO_2 is a renewable carbon source which is easily available in high purity, these new class of amphiphilic di-block polymers are considered as environmentally friendly macro-surfactants. Systematic phase behaviour studies revealed that the addition of the mPEG44-b-PBC10 polymer to a water - n-decane - $C_{10}E_4$ microemulsion only slightly increases the efficiency of the surfactant in solubilizing water and oil. The reason is the poor interaction between n-decane and the polycarbonate block. Using instead an oil which is a better solvent for the polycarbonate block, the mPEG44-b-PBC10 polymer were found to indeed strongly increase the efficiency of C10E6 to form water - hexyl methacrylate - $C_{10}E_6$ microemulsions. The SANS studies revealed, that the addition of mPEG44-b-PBC10 to the system water - hexyl methacrylate - $C_{10}E_6$ leads firstly to increasingly negative values of fa, which indicates a much higher ordering of the structure. However, when the amount of mPEG44-b-PBC10 is increased, the fa value becomes less negative again, which might be an indication that also hexyl methacrylate is not the optimal solvent for the polycarbonate block.

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IN42 Molecular diffusion in cell-mimicking droplets depending on size and shape

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Micrometric confinement by biomembranes is a characteristic structure in cells and intracellular organelles. The biomembrane does not only serve as the compartment boundaries but also play important roles by interacting with functional biomolecules. We have been studying such biomembrane functions by using liposomes on their deformation [1] and interactions with proteins [2]. Such membrane confinement should also contribute to molecular diffusion in cells, which is essential to various cellular activities.

In this study, we aimed to investigate the membrane confinement effect on molecular diffusion. For this purpose, we used cell-sized droplets covered with a lipid layer as a cell model [3] and analyzed molecular diffusion inside by fluorescence correlation spectroscopy (FCS) [4]. Compared to the liposomes, the droplets have the advantage of easier control of (i) degree of macromolecular crowding, (ii) droplet size R, and (iii) droplet shape. By changing these parameters, we can separate ?confinement effect? and the ?small volume effect? on molecular diffusion under macromolecular crowding.

We studied molecular diffusion of green fluorescent proteins (GFP) and fluorescent molecules (Rhodamine 6G and TAMRA) in linear chain polymer: poly(ethylene glycol) (PEG) and globular protein: bovine serum albumin (BSA) solutions. The diffusing molecules show delayed diffusion within the small crowding droplets than bulk solution regardless of the type of diffusive molecules and crowding polymers. In addition, the diffusion of crowder polymers also slowed down in the situation. To clarify the cause of the slow diffusion, we measured the diffusion coefficient inside of disc-shaped droplets and compared to the spherical droplets with the same volume. Surprisingly, the slow diffusion was observed inside the disc-shaped droplet with a larger volume than the spherical droplet. We also confirmed that the bulk solution with lipid membrane interface (i.e. no confinement) does not depend on the distance from the membrane for the diffusion coefficient. Taken together, we found that the main cause for producing slow diffusion under a macromolecular crowding is the membrane confinement rather than the small volume [5].

It should be noted that the GFP diffusion inside small droplets containing aged PEG, the diffusion coefficient of GFP became polydisperse and increased as the droplet radius R decreases [6]. It suggests that the crowding of PEG inside small droplets becomes heterogeneous, which is also observed for the above-mentioned experiments. Therefore, membrane confinement of the crowding polymer solutions alters the polymer-polymer interaction, which might cause slow diffusion and also fast diffusion depending on the altered interaction. The micrometric confinement and the macromolecular crowding would be key parameters that synergistically control the cell activities.

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IN43 Membrane adhesion of liposomes increases membrane tension and regulates in-membrane molecular diffusion

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Membrane adhesion plays a key role in many multi-cellular processes such as tissue formations. The physicochemical properties of lipid membrane without adhesion have been studied using isolated liposomes as model cells [1, 2] but less explored for adhered liposomes due to the difficulties to form the adhered tissue-like liposome system. In this study, we investigate the effects of the mechanical characteristics of the tissue model liposomes compared to the isolated cell model liposomes. For this purpose, we formed adhered liposomes as a tissue model through a modification of the suspending solution [3] without the addition of adhering membrane proteins.

Laser tweeter was used to pull a membrane-adhered colloidal particle by avidin-biotin interaction to measure the membrane tension γ of the liposomes where no membrane-membrane adhesion. The colloid was pulled to length L then released to spontaneously retract to the initial position. The membrane tension γ is calculated from the beads retraction velocity [4]. As a result, we found that membrane tension rises about 6 times for the tissue model adhered liposomes than isolated cell model liposome.

To explain the increase of membrane tension γ upon the membrane adhesion, we assume that the membrane-adhered region cannot be stretched due to the strong interaction between the two membranes. To assess our hypothesis, the molecular diffusion of the adhered and no-adhered area was measured by fluorescence recovery after photobleaching (FRAP). The increase of diffusion coefficient D is found for tissue model adhered liposomes than the isolated liposomes. Therefore, the increases of the membrane tension γ and the diffusion coefficient D have a positive correlation in the membrane adhesion. These results support our hypothesis that the membrane adhesion limits the molecular diffusion in the adhered area resulting in increased membrane tension in the no-adhered area [3].

The membrane tension γ was plotted against the adhered area fraction S_{ad}/S_0. As expected, the membrane tension γ increases as the area fraction of the membrane-adhered region increase. This result matches with a reported simulation [5]. Slow lipid diffusion induced by membrane adhesion protein has been reported and the mechanism is ascribed to increased friction between the membrane and the substrate [6]. Our simplified model also indicates a similar effect. Therefore, these changes might be due to the restricted lipid molecules diffusion in the membrane adhesion area.

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IN44 Surface charging kinetics reveals reaction mechanism

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Many surfaces obtain their charge by the reactive de- or adsorption of ions, but for many surfaces these reactions are ill characterized. We show that by studying charging kinetics one can extract the reaction mechanism, valency of reactive ions and reaction rate. This information is contained in the extent to which the charged surface attracts and repels ions. This effect is described by coupling Langmuir kinetics to Poisson-Boltzmann theory, allowing us to derive an analytic solution and a relation between decay rate and surface charge.

IN45 Rapid confocal imaging of vesicle-to-sponge phase droplet transition in dilute dispersions of the C10E3 surfactant

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The lamellar-to-sponge phase transition of fluorescently labelled large unilamellar vesicles (LUVs) of the non-ionic surfactant triethylene glycol mono n-decyl ether (C10E3) was investigated in situ by rapid confocal laser scanning microscopy (R-CLSM).

For that purpose, stable dispersions of dilute micrometer-sized C10E3 LUVs (0.003 w/w) were first prepared at 20C, and then quickly heated at three different temperatures (temperature quenching), i.e. close to, or above the lamellar-to-sponge phase (Lα-to-L3) transition temperature. For the lowest T-quenching (28C), we observed how primary LUVs evolve over minutes towards multilamellar objects with increasing number of membranes and local membrane concentration. In comparison, T-quenching at 30C or 35C led to much faster kinetics of membrane transformation. As a consequence, most of the intermediate structures seen at 28C were never observed, and LUVs were evolving over a few seconds towards sponge phase (L3) droplets.

The observed shape transformations with temperature can be interpreted in the light of the known property of those class of surfactant, i.e. their monolayer curvature H_0 decreases with increasing temperature. As a consequence, when temperature increases bilayers have to minimize their bending energy, evolving through new shapes that incorporate saddle points.

If the kinetics of temperature increase is low (T-quenching 28C), 'inter'-fusion of neighboring objects takes place, resulting in the overall increase of the object average size, rapidly followed by shape transformations , corresponding mainly to a first step towards a 'red blood-cell'-like structure, i.e. a biconcave disk shape object, then followed by an invagination step leading to a smaller, onion-like, object with an increased density of bilayers. This process is 'slow', with a typical time of a few seconds. Besides, for T-quenching at 30 C and 35 C, i.e. in case of a higher rate of increase of the temperature in the sample, corresponding to a stronger and faster decrease of H_0, bilayers do not only undergo the previous shape transformations based on inter-fusion events but also rearrange through 'intra'-object fusion processes, leading to a even more dense organisation of the bilayers. We show a wide collection of confocal images that help to build that scenario of the Lα-to-L3 phase transition, at the level of individual, diluted bilayers. We further demonstrate that it is possible to measure the bending modulus of the C10E3 bilayer through the analysis of the spatial and temporal fluctuations of a part of membrane, using both flicker noise spectroscopy, and spatial autocorrelation.

LI1 The Polymer Network of the Cytoskeleton affects Intracellular Phase Separation in Eukaryotic Cells

BOEDDEKER, Thomas (ETH Zurich); DUFRESNE, Eric (ETH Zurich); ROSOWSKI, Kathryn A. (ETH Zurich)

Stress granules are membrane-less organelles that form in eukaryotic cells as a response to harmful external cues. As such, they are of special interest in biology and medicine. Stress granules show liquid-like behavior and are thought to form transiently through intracellular liquid-liquid phase separation. The cytoplasm, however, is a very complex, active fluid and the formation and growth of these granules occur in the polymer network of the cytoskeleton. Previous results by our group on liquid phase separation in an artificial polymer network show that the network effects both formation and growth of droplets. Here, we present experimental results that suggest that similar mechanisms are at play in the case of stress granule formation and growth in living cells. Preliminary data indicate that network density correlates with the granule size and heterogeneities within the cell introduce directionality to the dynamics of the granules.

LI2 Enhancing lipid extraction from micro-algae suspensions using depletion flocculation and micro-fluidics

BOEK, Edo (Queen Mary University of London (QMUL)); TAGHI, Naoual (Queen Mary University of London)

The extraction of lipids from micro-algae suspensions has become a promising alternative to fossil fuel recovery. In addition, microalgae are established commercial sources of high-value chemicals for the pharmaceutical and nutrition industries. However, energy-efficient extraction of lipids from algal cells continues to be a major problem. Due to increasing demands for microalgal biomass and products originating from microalgae, large-scale production systems are required. However, current microalgal production technologies are not cost-effective and are limited by harvesting biomass.

First, cell separation is difficult because of the low sedimentation velocity of microalgae, their colloidal character with repelling negative surface charges, and low biomass concentrations in culture broths. Therefore large volumes need to be processed in order to concentrate the cells. Flocculation is one of the most efficient methods for harvesting microalgal biomass. To the best of our knowledge, only *enthalpic* flocculation methods have been described in the literature, using positively charged poly-electrolytes to flocculate the negatively charged algae in the algal suspension [1]. Here we report, for the first time, on the use of *negatively* charged poly-electrolytes, including carboxy-methyl-cellulose (CMC), to induce flocculation of the negatively charged algae, based on *entropic* depletion forces [2].

Second, and equally important, energy-efficient extraction of lipids from algal cells is an outstanding problem. In the literature, several methods have been proposed to enhance lipid extraction, including cavitation, pulsed electric fields leading to electroporation, and chemical hydrolysis [1]. Here we report novel micro-fluidic methods and micro-fabrication techniques to stress the algal cells in order to enhance lipid extraction.

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LI3 Adhesive interactions under flow at blood cell/vascular wall mimetic interfaces

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The immune or inflammatory response involves the recruitment of circulating blood cells to the vascular wall. A central player in such process is the so-called endothelial surface layer (ESL) lining the luminal surface of blood vessels, which displays signaling and adhesion molecules allowing for specific binding under flow of white blood cells. The ESL is a soft and micron-thick macromolecular scaffold comprising hyaluronic acid (HA) as an integral constituent. In addition to its contribution to the mechanical properties of the ESL, HA provides binding sites for the receptor protein CD44 displayed at the surface of flowing leukocytes. While CD44/HA interactions are recognized to be involved in the early stages of cell recruitment, the question of how specific binding, ESL compliance and flow strength orchestrate to allow for cell/wall adhesion is far from being elucidated.

In this context, we propose an in vitro approach that combines surface functionalization, microfluidics and 3D microscopy, allowing us to investigate in details the interplay between biochemical interactions and physical/mechanical parameters [1]. We design well-controlled cell mimetics bearing CD44 receptors and probe their behavior under flow past surfaces displaying HA layers that recapitulate the typical thickness and softness of the endothelial surface layer. We thus investigate how ligand/receptor density, flow strength and HA layer softness affect the rolling dynamics of flowing particles in the presence of specific adhesive interactions relevant to cell homing to the vascular wall.

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LI4 Active junctions as a pathway to stress generation in morphogenesis

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During the early stages of embryonic development cells spontaneously organise to exert contractile mechanical forces, resulting in convergence-extension flow of the entire tissue. Current models assume pre-patterning of molecules that control cellular junction contractions leading to the preferred direction of tension and flow.

Here we present a model of self-amplifying contractile confluent cell sheets that couples myosin activation to local junctional tensions thus allowing for the emergence of the directionality of contractions. This active mechanics leads to the spontaneous formation of tension chains observed in experiments.

We show that for a patch of 4 cells, the model features spontaneous active T1 transitions (i.e., against the external tension) when the surrounding passive matrix is stretched. Importantly, active T1 transitions are resolved via the sole mechanical forces without enforcing symmetry breaking of the myosin distribution. When all cells are activated, such active T1 transitions cooperatively lead to tissue rearrangements closely resembling experimentally observed convergence-extension flow.

We also show the influence of the relevant parameters of the model over the timescales involved in the resolution of the T1 using statistical tools to study the tissue deformation [1].

[1] Discrete rearranging disordered patterns, part I: Robust statistical tools in two or three dimensions Franois Graner (LSP), B. Dollet (LSP), Christophe Raufaste (LSP), Philippe Marmottant (LSP)

[We acknowledge funding from the UK BBSRC through grants BB/N009150/1, BB/N009150/2 (SH,LC,IDC) and BB/N009789/1 (RS,CJW)]

LI5 Toward theoretical model for cell blebbing

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Cell blebbing corresponds to the dissociation of cell membrane from the inner cellular network as result of internal stresses. Therefore, it represents the instability of the connection between the membrane and actin cortex. We employ a coarse-grained cell model to study cell blebbing for a number of involved parameters, including membrane rigidity, cytoskeletal stress, and binding strength between the membrane and bulk cytoskeleton. Furthermore, theoretical model for the detachment of bound solid surfaces is extended in order to include the effect of deformable cellular structures on the blebbing process.

LI6 Optimising Membrane Uptake of Patchy Nanoparticles by Artificial Evolution of Coarse Grain Simulations

FORSTER, Joel (IPLS, University College London); SARIC, Andela

Many membrane deforming nanoparticles used seek to mimic the entry method of viruses found in nature which involve the binding of membrane sites by attractive ligands on the surface of the foreign body being accepted. Previous studies have suggested that ligand position and mobility can impact the uptake of a particle by the cell, however a complete understanding of the structural features that govern uptake remains incomplete. In this study, the spatial distribution of these ligands was investigated as well as the large scale structures they give rise to. Coarse grain simulations of the cellular membrane, and of a model nanoparticle were used in the context of an evolutionary algorithm to explore the parameter space governing ligand placement and seeking optimal ligand patterning to enable cell entry across various ligand population sizes. Analysis of the neighbourhoods of the ligands across designs suggest that arrangements of ligands into low density but connected networks is optimal at low ligand numbers and that in this regime, much like artificial communication networks, small-world properties are advantageous. Future work aims to fully characterise the parameter space which encodes for these particles to determine the design rules which govern passive endocytosis and develop a tool for computer aided rational design of membrane deforming structures.

LI7 Dynamical rheological properties of in-silico epithelial tissue by vertex models

ISHIMOTO, Yukitaka (Akita Prefectural University); TOYOSHIMA, Takuya

Many biological systems including humans are made up of various cells. In addition, cells of a specific type gather together to form tissues, and organs are organized as an aggregate of multiple tissues. One of the tissues constituting organs is epithelial tissue. Epithelial tissue is composed of epithelial cells, and almost without exception the surface inside and outside the body is covered with epithelial tissue, many of which are monolayered. Mathematical models expressing morphogenesis of epithelial tissue have been developed by many researchers. One of the models, vertex model (VM) [1] discusses tissue growth by polygon approximation of cells, but it does not take account the curvature of cell boundaries. Therefore, Ishimoto, et al., developed the bubbly vertex model (BVM) [2] introducing the curvature into this model and studied the tissue growth of the epithelial tissue.

Morphogenesis of epithelial tissues is nothing but the formation of multicellular mechanical structures by intercellular communication and intracellular activities. Computer-aided elucidation of such formation mechanisms has been awaited for further applications. However, correspondence between existing simulation models and epithelial tissues has not been established due to the complexity of even the basic physical properties of the tissues. In addition, the properties may vary depending on morphogenetic stages and the affiliated organ.

In this study, we focus on two mathematical models of epithelial tissue: the cell vertex model and the bubbly vertex model. We analyze the rheological properties of the models by simulation and aim at finding a correspondence with actual viscoelastic epithelial tissues. Concretely speaking, we analyze the dynamic behavior of the tissue model which hexagonal shape is considered the ground state [3]. As a simulation evaluation method, rheological characteristics of epithelial tissues are expressed by complex modulus and its mechanical characteristics are evaluated. In our simulation, an isotropic stress given by sine waves of different periods are applied onto the tissue boundary, and the resulting area strains are calculated. Thereafter, the phase differences are calculated from the applied stress and so are the area strains.Thus, the rheological characteristics are evaluated.

From our results, viscoelasticity of epithelial tissue was confirmed in a specific frequency range in both simulations of VM and BVM. In these models, when we ran the simulation with changing the elastic modulus of cell boundaries, no significant change in the dynamic behavior was observed in a low frequency region regardless of the elastic modulus, however, only in the BVM, the dynamic behavior exhibits nontrivial changes in a high frequency region.

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LI8 How different chemical treatment affects mechanical fingerprint of *P. fluorescens* biofilms

Jinju Chen (Newcastle University); Sam Charlton (Newcastle univ), Saikat Jana (Newcastle univ), Tom Curtis (Newcastle univ)

Biofilms are bacteria community encased within a self-secreted extra polymeric matrix (EPS) composed of carbohydrates, proteins and extracellular DNA. The multifaceted role of EPS confers protection against external challenges contributing to antibiotic resistance and hydrodynamic inefficiencies. Biofilms are also harnessed advantageously to reduce dependence on energy intensive water remediation systems and as a potential source of energy generation through biological fuel cell technology. The understanding of biofilm mechanics is important for us to control and manage biofilms. Current work on biofilm mechanics has mainly been limited to linear viscoelastic regime. But biofilm deformation in most real world cases may take place beyond the linear viscoelastic regime. However, there is lack of comprehensive study to quantify the non-linear rheology of biofilms. With advancements in rheometer hardware, large amplitude oscillatory shear (LAOS) tests are viable to investigate non-linear viscoelastic behaviour and yielding of soft matter. Therefore, this study aims to establish appropriate protocols to investigate non-linear viscoelastic behaviour of P. fluorescens and employ several powerful analytical tools (such as Chebychev stress decomposition method) to reveal the nonlinear characteristic effects of *P. fluorescens* biofilms treated by different chemicals (e.g. urea, $FeCl_2$, $CaCl_2$). It has shown that the urea cause significantly different mechanical fingerprint compared to the rest. It has revealed that both EPS polymer physics and bacteria packing are important for the overall mechanical signature of the biofilms. The key findings in this study are valuable for us to understand the mechanics of biofilms as living soft matter.

LI9 Chemical modulation of phage stability

KSIĘŻARCZYK, Karolina (Institute of Physical Chemistry of the Polish Academy of Sciences); RICHTER, Łukasz; TAKENAKA, Shigeori; HOŁYST, Robert; PACZESNY, Jan

The development of agents for stabilization of bacteriophages will have positive impact on vaccination programme in underdeveloped countries or biocontrol methods in biotechnology industry. Moreover, phages might be drug of last resort in number of cases induced by antibiotic resistant bacteria. It is noteworthy, that some species of bacteriophages are very similar to human viruses, and might be used as their biological models e.g. MS2 is the model of Rihnoviruses spp. While the large-scale of phage stabilization projects are based on genetic modifications of bacteriophages genome, in our studies, we focused on chemical methods of stabilization, by using special synthesized molecules as well as natural compounds.

Four bacteriophages, i.e. T4 (Myoviridae), T7 (Podoviridae), MS2 (Leviviridae) and M13 (Inoviridae) were tested for their thermal stability. For every temperature (37, 40, 50, 55, 60, 65, 70?) the decrease of active phages was determined. Physiologically, we observe that even slightly increase of temperature may cause destabilization of capsid structure, as proteins are held together by non-covalent interactions, easy to dissect. Furthermore, the biological and physiological variety of bacteriophages contributed to the differences in the ratio of phage concentration decrease (e.g. T4 phages were able to survive in 50? for more than 2 weeks when MS2 phages were vanishing after 48 hours). Depending on phages, an optimal condition for an effective application are different, and the effective and fast method for thermal stabilization is eligible. We studied PEG chain flanked with two intercalator domains which can bind to phage DNA, which empowered whole capsid. It turned out that after addition of our synthesized compound - APEG (acridinyl poly (ethylene-glycol) - the stability of phages increased significantly. The amount of APEG was very low (3ng/ml), which makes the method widely applicable. Our method is faster and cheaper than used to date.

LI10 Boosting of the diffusion of soft nanoparticles in confined media

LATREILLE, Pierre-Luc (Université de Montral); Universit de Montral

The understanding of colloids dynamics in heterogenous and confining media has direct implications on nanotechnology research, material science and nanomedicine. In the latter, soft nanomaterials have received increased attention because of their deformable nature and their greater in vivo performance to cross biological membranes or deeply penetrating tissues. However, the link between deformability and those performances is not obvious. Most of these observations were produced in vivo and were not supported by experiments performed in a controlled environment. The only solid evidence of shrinking or deforming nanoparticles (NPs) is by applying external forces or stimuli. So, the idea that soft NPs spontaneously shrink in a confining environment, therefore improving its ability to cross biological membranes or penetrating tissues, must be questioned. Assuming that biological matrices have a gel structure, we decided to characterize the dynamics of hard and soft NPs and compare their effective diffusivity in these effective media. Agarose was used to produce gels with fibrillar structures that are found in complex organisms making it the simplest relevant gel to study. Hard NPs made from gold capped with poly(ethylene glycol) and soft hydrogel NPs made from poly(N-isopropyl acrylamide) were introduced in agarose gels and their diffusion coefficient was measured by differential dynamic microscopy (DDM). Different sizes of NPs (r_H = [20, 120] nm) were used as well as different agarose concentration spanning from (0.05 to 0.1% w/w) – viscous solution – to (0.5 to 1% w/w) – gelled media. It was found that in agarose solutions, diffusion of hard and soft NPs was similar and follows the Stokes-Einstein equation, where diffusion is governed mostly by the solution viscosity and particle size. However, in agarose gel, soft nanoparticle's diffusion is significantly faster, up to 2 order of magnitudes, compared to hard spheres. Using the Ogston model of diffusion (stochastic approach of NPs motion through randomly oriented cylinders), soft NPs were predicted to shrink half their size. This result was consistent with the Dhont diffusion model (incorporating hydrodynamic and electrostatic contributions to the diffusion) which also predicted a shrinkage of $\approx 50\%$ of the NPs. We proposed that the shrinking of the particles in gelled agarose is due to the strong overlapping of the electrostatic double layers from the particles and the agarose fibers forming the gel. Finally, we show that soft NPs can spontaneously adapt by changing their size and consequently boosting their diffusion in confined media. We also show that this is best explained as an electrostatic phenomenon. This mechanism suggests that soft NPs can adapt to confinement and penetrate deeper dense tissues.

IN11 Physical mechanisms of cell-cell cohesion and aggregation in liquid suspensions of bacteria

MELAUGH, Gavin (University of Edinburgh); ALLEN, Rosalind (University of Edinburgh); MARTINEZ, Vincent (University of Edinburgh); WOZNIAK, Dan (Ohio State University); HOWELL, Lynne (University of Toronto)

Multicellular bacterial aggregates are found in many clinical and industrial environments. These range from the cystic fibrosis lung, where they are detrimental, to the secondary treatment process in wastewater treatment (WWT), where they are beneficial. Understanding the biological and physical mechanisms by which the cells clump together to form such aggregates is therefore crucial for developing methods for eradication (clinical) on one hand, and optimisation (WWT) on the other. Research in this area is almost solely done in the context of biofilm formation, in which the bacterial cells are associated with a surface and follow a well-defined life cycle, yet many of the bacteria in these environments have a tendency to aggregate in the bulk liquid (or viscoelastic media) much like in a colloidal bath. Thus, to gain deeper insight into the factors driving aggregation in these systems, we have adopted a soft matter physics approach by considering these suspensions of bacteria as model living systems for active self assembly.

Using the model biofilm-former *Pseudomonas aeruginosa*, we have performed a series of simple experiments identifying the biological and physical mechanisms driving aggregation in bulk liquid. Our results show that many factors such as cell motility and intercellular signalling play a role in aggregate formation, but the crucial factor driving aggregation is polymer induced cell-cell cohesion. Our results highlight two aggregation regimes: 1) during the growth phase, where the polysaccharide PSL, mediates cohesion between cells via a polymer-bridging interaction that is strongly irreversible, and 2) during starvation conditions, where cell-cell cohesion is mediated by the production of extracellular DNA resulting in aggregates that are quite different to those formed by PSL.

IN12 Understanding the Tip Tracking Mechanism of End-Binding Proteins on Microtubules

MOSBY, Lewis (The University of Warwick); POLIN, Marco (The University of Warwick); STRAUBE, Anne (The University of Warwick); ROTH, Daniel (The University of Warwick)

Microtubules are cylindrical structures that constitute one part of the dynamic cytoskeletal network inside cells, and which act as tracks for the intracellular transport of cargo by motor proteins. Growing microtubules can recruit specialised end-binding proteins (EBs) that bind preferentially (and for longer) to the specific conformation of GTP-bound tubulin at the microtubule tip [1,2]. Transient binding between cargo (such as vesicles) and these tip tracking EBs has been shown to result in the directional transport of cargo within cells. In order to understand the exact mechanism by which EBs couple microtubule polymerisation to cargo motion, both the processes of EB-microtubule and cargo-EB binding must be understood. Here, we combine modelling and experiments to study the EB-microtubule interaction. Our results suggest that elongated EB dwell times at the microtubule tip are due to the existence of distinct 'weakly' and 'fully' bound states that can facilitate the biased diffusion of EBs (and therefore cargo) inside cells.

Reducing the dynamics of the EB-microtubule binding to a pair of coupled, one-dimensional Fokker-Planck equations allows the derivation of analytical forms of the average dwell time, effective diffusivity, and stationary state distribution for bound EBs. In contrast with previous studies [1,2], our experimental data clearly displays that EBs have two characteristic unbinding timescales, which our model predicts are due to the presence of both a weakly and a fully bound state. Similarly, comparison between analytical and experimental distributions suggests that elongated dwell times at the microtubule tip are due to a tip-localised increase in the transition rate into the fully bound state. Further experiments involving monomeric EB constructs are helping to clarify whether the two bound states are the result of an intermediary electrostatic EB-microtubule interaction, or whether each one of the two microtubule binding sites on a single EB can bind independently to the microtubule.

Extension of the analytical EB binding model to consider cargo permanently engaged with multiple EBs results in a dwell time distribution with two distinct regions: for small numbers of cargo-bound EBs the evolution of the dwell time is heavily dependent on the initial binding state of the system, whereas for larger numbers of cargo-bound EBs the dwell time grows exponentially.

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LI13 Fracking Bacteria: The mechanical origin of submerged colony morphology

MUIR, Edward (University of Edinburgh); WACŁAW, Bartlomiej (University of Edinburgh); POON, Wilson (University of Edinburgh)

Escherichia coli submerged in agarose gel grow into ellipsoidal colonies, reminiscent of “Penny shaped” hydraulic fractures. In an analogous system, silicone oil is injected into the same gel, bubbles with the same morphology are created. This suggests that colony morphology has a purely mechanical origin, rather than biological. Time lapse single plane illumination microscopy (SPIM)is used to measure deformations around the growing colonies. Measuring these deformations reveals that the governing mechanism of colony morphology is fracture, the internal pressure of a growing colony fractures the agarose in a single “Penny shaped” plane. Thus, the fundamentals of linear elastic fracture mechanics, along with some modification for the small scale of the colonies, is shown to predict the morphology of submerged *Escherichia coli* colonies.

LI14 The interaction between T4 bacteriophages and different polypropylene surfaces

PASZKOWSKA, Karolina (Institute of Physical Chemistry Polish Academy of Sciences); KSIEZARCZYK, Karolina, RICHTER, Lukasz, HOLYST, Robert, PACZESNY, Jan

The quality and type of plastic labware is usually ignored as a factor influencing scientific results. However, sometimes it may happen that unexpected errors occur in biological measurements (e.g. in enzymes activity or quantity of DNA). In our research we show that, surprisingly, these errors may be caused by the brand of used plastic labware.

Here we show studies on T4 bacteriophage, which host is Escherichia coli. It is very popular and well described bacterial virus which is broadly used in virological laboratories. Two types of plastic tubes were tested: eppendorf tubes (1.5 ml) and falcon tubes (50 ml), all made of polypropylene (PP). We determined with a very good repeatability, which of them are ‘safe’ (i.e. not causing significant decrease in phages activity) and which are not. As a control, we used glass tubes, which did not bring any effect on virus activity. In the case of ‘unsafe’ eppendorf tubes, the decrease of virulence was observed in relatively high temperature (50C) (2 orders of magnitude down after 3 days and complete deactivation after 7 days of incubation). In ‘unsafe’ falcon tubes, the strongest decrease of the number of active phages was seen when the tubes were stirred vigorously (640 rpm) (5 orders of magnitude down after 5h of stirring) and the effect decreased with decreasing stirring speed. Both without stirring (falcons) and at room temperature (25C, eppendorfs), phages activity remained stable for long time (up to 7 days). What is more, it was observed that small amounts of surfactant stabilizes phages against stirring and/or heating.

We performed SEM and AFM measurements to observe plastic surfaces after the experimental processes. These measurements confirmed that after fast stirring active phages are present on the tube wall, even when they are no active phages in the suspension.

We propose a hypothesis, that T4 phages are physically adsorbing on plastic walls. T4 phage might be attracted electrostatically to the polymer by its positively charged tail fibers. During stirring or heating the tube, phages are transported faster towards the tube wall and the process of attraction is enhanced. The ‘safety’ of some brands of tested PP tubes could be caused by special additives to the polymer suspension. They may be present at the inner surface of the tubes, restricting phages from adsorption.

LI15 Nonlinear Poisson effect in critical mechanical networks

SHIVERS, Jordan (Rice University); ARZASH, Sadjad (Rice University); MACKINTOSH, Fred (Rice University)

Fibrous networks of stiff athermal biopolymers such as collagen, a major structural component of the extracellular matrix, have been shown to exhibit anomalously large apparent Poisson's ratios, i.e. significant transverse contraction under incremental applied longitudinal extensional strains. We show that this effect can be understood in the context of a macroscopic mechanical phase transition from a bending-dominated regime to a stretching-dominated regime at a critical applied extension controlled by the network connectivity. We measure this effect using a variety of 2D and 3D model network structures and propose a phase diagram governing the transition as a function of connectivity and strain.

LI16 Quasi-two-dimensional dispersion dynamics of protein monolayers

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Understanding the dynamics of interacting globular proteins embedded in a three-dimensional fluid but confined to a planar monolayer is of great challenge in (biological) soft matter science. The interplay of two-dimensional translational particle motions and solvent-mediated three-dimensional hydrodynamic interactions in these quasi-two-dimensional (Q2D) systems gives rise to peculiar effects such as the anomalously strong enhancement of large-scale collective particles diffusion. Using the multiparticle collision dynamics (MPC) simulation method, we explore hydrodynamic and direct interaction effects on the Q2D translational and rotational protein diffusion in a broad range of time scales, from very short times where the particles dynamics is affected non-instantaneously by sound propagation in the fluid and transversal momentum diffusion, to long times where the hydrodynamic interactions are fully developed and non-retarded [1]. The proteins in the monolayer are modeled as Brownian spheres interacting directly via a pair potential consisting of competing short-range attraction (SA) and long-range repulsion (LR) parts that apply to protein solutions under low-salinity conditions. We analyze the concentration dependence of the collective diffusion coefficient at small and non-small wavenumbers, in conjunction with mean-squared displacements and real-space van Hove functions characterizing self- and collective diffusion. To reveal the development of inter-protein hydrodynamic interactions by sound propagation and vorticity diffusion, we compute velocity auto-correlation and cross-correlation functions and analyze the associated wave-vector dependent current correlation functions.

[1] Z. Tan and G. Nägele, work in progress.

MA1 Autonomous analysis of confocal images: using machine learning to recognize bijels

GOULD, Emily (University of Edinburgh); MACMILLAN, Katherine (University of Edinburgh), CLEGG, Paul (University of Edinburgh)

Bijels are becoming widely researched in soft matter, in terms of both new applications and simpler methods of synthesis. However, little work has been done to improve the ease with which we can identify whether or not a sample is, indeed, a bijel. This is a particularly relevant question for investigations into novel synthesis methods, where there is no guarantee that a bijel will have successfully formed.

We are developing a protocol using machine-learning techniques to allow the identification of a bijel from a single image. We use confocal data and classification judgements from previous bijel experiments, and process them in order to obtain parameters that may be useful for bijel identification, such as features of the autocorrelation function. Our approach is also capable of including composition information from the experiments into the classification process.

We then use some of these parameters to categorise images into bijel and not-bijel, using machine-learning algorithms. The algorithms allow us to identify which parameters are key for identifying the bijel, as well as generating a model that can be used to quickly and easily categorise future images from new samples. We compare several machine learning algorithms as well as an array of possible parameters, in order to achieve the lowest error rate possible when classifying bijels.

MA2 Dynamics of turbid colloidal suspensions using Differential Dynamic Microscopy

MARTINEZ, Vincent Arnaud (School of Physics & Astronomy, The University of Edinburgh); NIXON-LUKE, Reece (RMIT); ARLT, Jochen (University of Edinburgh); POON, Wilson (University of Edinburgh); BRYANT, Gary (RMIT)

We investigated the capability of Differential Dynamic Microscopy to characterise the particle dynamics of turbid colloidal suspensions based on standard microscopy. We measured the Intermediate Scattering Function (ISF) of polystyrene microsphere suspended in water over a range of concentrations, turbidity, optical path, and over 5 orders of magnitude in time-scales. We found the appearance of a short-time process as turbidity is increased, which we associated with multiple scattering. The long-time process corresponds to the particle dynamics from which particle-size can be estimated in the case of non-interacting particles. Additionally, we compared the results to those obtained from both Dynamic Light Scattering (DLS) and Two-colour Dynamic Light Scattering (TCDLS). The latter allows for suppression of multiple scattering for moderately turbid suspensions. We found that DDM can obtain reliable particle size at up to 10 times higher particle concentrations than TCDLS.

MA3 Nanostructure of particles revealed by SAXS/WAXS

RODRIGUES, Sergio (Xenocs SA); PANINE, Pierre (Xenocs SA); FERNANDEZ MARTINEZ, Manuel (Xenocs SA); DESVERGNE-BLENEAU, Sandra (Xenocs SA); NEWBY, Gemma (Xenocs SA)

Study of particles having nanometer scale organization is a very broad field of research. In the case of solid particles, it has been an active domain for decades, leading to interesting properties for use in electronic, biological and optical devices [1, 2]. In the case of soft materials, self-assembly of asymmetric molecules (surfactants, phospholipids?) has led to describe a hierarchical organization as such as liposomes under various forms, uni- or multi-lamellar vesicles and more complex phases. Besides the well-known drug delivery application of liposomes, recent findings have shown interest in the field of functional food [3]. The common point between these applications is their capability to be described in detail by small angle x-ray scattering. Beyond the particles sizing and structure, the capability to reveal the interactions between particles in and with the suspending media is also of interest. The coating of particles is one of crucial point leading to improved stabilities. It is therefore of high interest to be able to reveal finely its structure. On this paper we review the characterization of various types of nanosized particles using small- and wide-angle X-ray scattering (SAXS and WAXS). The main result, besides the particle size and size distribution, is the presence of a structure factor in the SAXS region and at the same time the presence of crystalline peaks in the WAXS regime that can be related to the stabilizing coating of the particles. This will demonstrate the capabilities and advantages of simultaneous SAXS/WAXS data collection on the Xenocs equipment.

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2. Shi S. and Russel T.P., Adv. Mater 1800714 (2018)
3. Chaves et al, Colloids and Surfaces A, 520, 112-121 (2018)

MA4 Measuring nanoscale properties of water capillary menisci

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Water menisci are present in most nanosystems in ambient conditions and can play a critical role in many different physico-chemical processes. Therefore, they have been extensively studied, particularly with nanoscale probing tools such as the atomic force microscope (AFM). However, the violent forces due to meniscus nucleation prevent the controlled use of such instruments since they often produce an irreversible dive of the AFM tip onto the substrate, known as the ?jump-to-contact? mechanism, which render the acquisition of the complete tip-sample interaction curve impossible. This means that capillary bridges studies are frequently performed without controlling critical parameters such as a defined geometry of the nanocavity. By using the technique of Force Feedback Microscopy (FFM), which adds a feedback mechanism to the conventional AFM instrument it is possible to stabilize the tip position and avoid jump-to-contact, which enables the measurement of the complete tip-sample interaction curve. We measured the condensation time and distance of these menisci by performing a series of force-distance curves and recording the tip-sample condensation distance dependence on the approach speed. This experiment attempts to clarify the disparity observed in recent studies concerning the formation of capillary bridges, especially regarding its nucleation time. By allowing full control of tip-sample distance and cavity geometry during the nucleation of the menisci, we believe the FFM may provide further insight into still unanswered issues about the behaviour and formation mechanism of this ubiquitous phenomenon.

MA5 Measuring the dynamics of soft matter using coherent X-ray radiation

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One tool for the investigation of soft matter sample systems is synchrotron radiation, which allows probing inter alia optically opaque samples or the bulk of a soft matter system. While most synchrotron studies concentrate on the structure of soft matter systems on the length scale of some tenths to some hundreds of nanometers, the use of a partially coherent X-ray beam allows to additionally investigate sample dynamics by using X-ray Photon Correlation Spectroscopy (XPCS). One of the places to perform XPCS experiments is the Coherence Applications Beamline P10 at PETRA III, DESY, which is dedicated to coherent X-ray scattering experiments. Mostly, the beamline operates in the energy range of 5-17 keV. It offers several experimental setups - two of these setups are especially well suited for soft matter systems. On the one hand a SAXS/WAXS instrument, where the detector can be translated between 0 and 30° at a sample to detector distance of 5m. And on the other hand an ultra-small angle X-ray scattering (USAXS) setup, where the detector is positioned at a sample to detector distance of around 21 m. This long pathway allows it to use a large fraction of the coherent flux in an unfocused X-ray beam, while providing a fairly strong speckle visibility. This setup is therefore ideally suited for radiation sensitive samples such as most complex liquids, as the flux per sample area can be considerably reduced using a comparatively large X-ray beam. Both setups can be used in combination with a number of fully vacuum integrated sample inserts allowing for temperature control, tunable magnetic fields or nano-positioning of samples. If needed, this vacuum environment can be replaced by a variety of other experimental setups or custom sample environments. To illustrate the experimental possibilities, results on colloidal systems will be displayed – on the one hand an investigation of a charge stabilized colloidal system which approaches the glass transition, and on the other hand of a colloidal system in flow.

MA6 The Synthesis and Materials Properties of Aromatic Cation Liquid Crystals

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Discotic liquid crystals, made of disc-shaped molecules that are able to self-assemble into column structures, are of interest as directional charge transporting functional materials in electronics [1]. These charge transfer properties can be introduced by the addition of ionic species into the liquid crystal molecules, or aromatic regions in the molecular core [2]. These properties can be combined together by the use of a stable aromatic carbocation as the molecular core of a discotic liquid crystal. By the use of a Friedel?Crafts synthesis with aromatic ether molecules, we are synthesising cyclopropenium cations bearing pendant oligomethylyene chains with the charge distributed across an expanded aromatic core. We synthesised a family of liquid crystals of different lengths and with the positive charges balanced by a range of different counter anions. We are investigating the effect that these changes in the molecular structure have upon the phase behaviour of these different materials.

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MA7 Upgrades of the neutron backscattering spectrometer SPHERES

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The neutron backscattering spectrometer SPHERES (SPectrometer for High Energy RESolution) at MLZ is a third generation backscattering spectrometer with focusing optics and phase-space transform (PST) chopper. It provides high energy resolution with a good signal-to-noise ratio [Wuttke et al., Rev. Sci. Instrum. 2012]. SPHERES enables investigations on a broad range of scientific topics. It is in particular sensitive to the incoherent scattering from hydrogen and allows to access dynamic processes up to a timescale of a few ns. Hence it is well suited to investigate dynamics in various soft matter systems like polymers [Mark et al., Phys. Rev. Lett. 2017] or proteins [Stadler et al., Biophysical Journal 2016]. Selective deuteration of samples allow e.g. measuring the component dynamics in novel nano-composites [Bhowmik et al., Macromolecules 2014] or follow the mobility of water on the surface of tau proteins and their fibers [Fichou et al., PNAS 2015].

Different components of the instrument have been upgraded to further improve the instrument performance. Some recent years ago the PST chopper has been renewed. The new more compact one-wing chopper can be operated with the desired frequency with a crystal speed of 225m/s close to the optimum velocity for the phase space transformation. Together with the exchange of the chopper also the graphite deflector crystals on its circumference were replaced with ones of a higher reflectivity and mosaicity. Thanks to the increased velocity and the better deflector crystals, the intensity in most detectors had been doubled. Just recently the focusing neutron guide has been replaced with an elliptic guide. It had been optimized based on simulations, which also considered the new PST chopper. With the new elliptic guide another intensity gain at the sample position of about 30% was obtained. Together with the exchange of the focusing guide also a new background chopper has been installed about 2m upstream of the PST chopper to further reduce background. This will then also allow for a high signal-to-noise setup by eliminating every second pulse, albeit at the cost of intensity.

MA8 New opportunities for multi-speckle x-ray photon correlation spectroscopy at ultra-small-angles

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Over the last several decades, the X-ray Photon Correlation Spectroscopy (XPCS) has emerged as a powerful counterpart to conventional Dynamic Light Scattering (DLS) for the investigation of concentrated complex fluids [1]. The key advantages of XPCS are optically opaque systems can be studied without significant influence from the multiple scattering and the shorter wavelength of X-ray enables accessing the dynamics at large wave vectors or small size scales. In addition, multi-speckle analysis using a 2D detector is relatively straightforward that allows direction dependent dynamics to be probed. Nevertheless, applications of XPCS have been primarily restricted to slow dynamics in condensed matter systems due to limited coherent photon flux and frame rate of high resolution detectors.

The above-mentioned limitations can be overcome at ultra-small angles using a state-of-the-art pixel array detector such as the Eiger500k detector developed at Paul-Scherrer-Institute (PSI) [2]. The higher scattering power of typical samples studied by ultra small-angle X-ray scattering (USAXS) and the rapid acquisition rate of the detector together enable XPCS to probe faster times than diffusive motions (Brownian) in aqueous medium. Applications of ultra-small-angle XPCS (USA-XPCS) include fast advective motions in a hydrodynamic flow [3], active motions of self-propelled particulate systems [4], etc.

Here we present the first performance tests of the new Eiger500k single photon counting pixel detector at the TRUSAXS beamline ID02, ESRF, Grenoble (France) [5]. Together with the unique low q-range: 0.001 – 0.1 nm^{-1} i.e. length scales from m down to tens of nm accessible within one experimental setup, the fast high resolution Eiger500k opens a whole set of new applications studying particulate dynamics on a time scale of 100 s by multi-speckle XPCS, e.g. silica colloids. This will be further illustrated using examples of the phoretic dynamics of active colloids, velocity fluctuations in hydrodynamic flows etc. probed by USA-XPCS.

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MA9 Demonstration of a touch-responsive photonic laminate from cellulosic material and roll-to-roll processing

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Cellulose is the most abundant natural polymer in the world and has many derivatives. One such derivative is Hydroxypropyl-cellulose (HPC). Upon dissolution, HPC can self-assemble into a chiral nematic (ie. cholesteric) liquid crystal with a helical nanostructure, the periodicity of which leads to striking colours from Bragg reflection. This selective Bragg-reflection is highly sensitive to the application of pressure, termed mechanochromism, and renders HPC a responsive photonic material. Thus far, advances in understanding the mechanochromic properties of HPC have yielded few real-world applications, requiring both up-scaling and digital translation of its colour change. Indeed, the self-assembly of large molecule and nanoparticles should allow for the development of materials with novel properties. To date however, most self-assembled structures are demonstrated on very small areas and under well-controlled lab environments - not congenial to industry or commercial application. Presented here are roll-to-roll (R2R) manufactured metre-scale HPC laminates, produced by continuous coating and encapsulation of photonic HPC material. The result is a large area flexible film that changes colour when pressure is applied. As a demonstration, the pressure of a foot-imprint was mapped in real-time using a smartphone video. The HPC colour response was quantified with optical analysis of the hue-change during a known pressure application, as perceived by the human eye and digital imaging, and used to calibrate the real-world measurement. The real-time video allowed for frame-by-frame RGB pixel extraction to obtain the dynamics and motion signature of the foot imprint. For example, we observed that the subject places little pressure on their small toe as the colour change in this region was absent throughout the recording. The average RGB colour was calculated from squares of 10 x 10 pixels to minimise the effects of camera noise and small pixel-to-pixel variations. These average RBG values were then converted to corresponding hue-values for analysis. Overall, this demonstrator showed the ability to readout 2D pressure maps over time using a low cost mechanochromic HPC film and a mobile phone camera rather than arrays of pressure sensors that would be more expensive and complicated to integrate and analyse. However, this is just one demonstration and for any given application various parameters would need to be optimised, such as the processing parameters, lamination materials, active material specifications etc.. However what we have shown is that a self-assembled nanostructure can be utilised in a real-world environment and for practical use without the need for excessively complicated manufacture and interpretation. This was achieved through established techniques of continuous R2R slot-die coating and lamination processes, combined with the low cost and biodegradable photonic material that is HPC.

PO1 Experimental investigation of EVOH precipitation in a T-shaped microchannel

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One of the progressive methods of intravascular neurosurgery is embolization of brain cerebral arteriovenous malformations (AVMs) with the aim of complete filling of nidus. Ethylene-vinyl alcohol copolymer (EVOH) has emerged in the recent years as a new embolic agent. Optimization of the embolization procedure is very important for practical neurosurgery and is of considerable interest as the task of multiphase hemodynamics. An embolic composition based on EVOH in dimethyl sulfoxide (10%) was prepared and its flow in a microchannel with aqueous phase was investigated. The precipitation of polymer was visualized by using a microscope in a T-shaped microchannel made of SU-8 with a rectangular cross section with characteristic dimensions of 200x200 μm and 200x400 μm for the input and output channels, correspondingly. The length of the input and output sections was 5 mm. The flow rates of the liquids were set by double syringe pump. The embolic agent flow rate was varied from 1 to 30 μl/min, while aqueous phase flow rate was set in the range from 1 to 180 μl/min. Four main precipitation scenarios were revealed. The first scenario consists in uniform polymer precipitation along the entire channel length and its subsequent embolization. The second scenario is characterized by the growth of the filamentous structure, which can be deformed and carried away by the stream as a whole, which also leads to embolization. In the third scenario when the aqueous phase flow rate was higher than embolic agent flow rate the plug was formed near the junction. The last scenario showed a uniform precipitation of the polymer along the interface between aqueous and embolic phases which leads to the separation of the phases without subsequent embolization of the channel. The precipitation scenario map was constructed using flow rates of the aqueous and embolic phases. The change in the amount of precipitated polymer in the microchannel was analyzed at different flow rates of water and embolic agent over time based on a measurement of the average gray intensity in the image. It is established that the average time of embolization varies from 100 to 300 s. The experimental data obtained in the present work could be useful for the verification of numerical simulation of embolization process.

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PO2 Internal structure and dynamics of homogeneously and heterogeneously crosslinked PNIPAM microgels

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Thermoresponsive poly(N-isopropylacrylamide) (PNIPAM)-based polymer systems due to their reversible temperature induced volume phase transition (VPT), that is close to the physiological temperature, are of high research interest during last decades. Introduction of the crosslinker into the microgel network leads to the inhomogeneous internal polymer density distributions due to difference in transition temperate, i.e. thermal and 'frozen' inhomogeneities appear [1]. To investigate structure and dynamics of microgels with different internal homogeneities (from homogeneous to heterogeneous), PNIPAM microgels with N,N'-methylenebisacrylamide (BIS) as crosslinker prepared via precipitation polymerization and continuous monomer feeding were investigated by means of dynamic light scattering (DLS), small-angle neutron scattering (SANS) and neutron spin-echo spectroscopy (NSE). We report on the direct comparison of the internal structure of the microgel particles in dependence on the crosslinker concentration (0.5 - 5mol%), preparation process and initiator concentration. Moreover, dynamics investigation taking into account the presence of different types of internal inhomogeneities inside PNIPAM microgels are presented.

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PO3 Dynamics of poly(methyl methacrylate) chain in thin films during solvent annealing studied by neutron reflectometry

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he chain dynamics of poly(methyl methacrylate) (PMMA) in spin-coating films during solvent annealing was studied by neutron reflectometry (NR). The *in situ* NR measurement of the PMMA film exposed to the vapor of toluene showed that the absorbed solvent molecules homogeneously distributed in the spin-coated film and the solvent fraction increased to 0.35. In order to examine the dynamics of the PMMA chain, a five-layered thin film of deuterated PMMA (dPMMA) and hydrogenated PMMA (hPMMA) was prepared, each of which has a thickness of 20 nm. The diffusional motion of the PMMA chain can be examined as the rate of the increase of the interfacial width between the dPMMA and hPMMA layers. At first, the chain dynamics in thermal annealing at a temperature of 140$\circ$C was examined by the real-time NR measurement. It was found that the diffusion dynamics of the PMMA chain was strongly dependent on the depth from the surface: the polymer chain at the substrate was restricted, while the chain at the surface showed a large diffusivity. On the other hand, the depth dependence of the chain dynamics was weak in the spin-coated film in the solvent annealing process. Whereas the ratio of the diffusion constants of the PMMA chain at the surface and substrate was 50 in thermal annealing, the ratio in toluene vapor was as small as 2. Therefore, the solvent annealing provides sufficient mobility to the polymer chain near the substrate. This result indicates that the solvent annealing method enables the equilibration of a spin-coated polymer film from the surface to the substrate interface.

PO4 Semiflexible Polymers in Spherical Confinement

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Semiflexible macromolecules find various applications as versatile materials, in particular due to their possible liquid crystalline order, and are also important constituents of living matter. We studied the ordering of such stiff macromolecules confined in spheres by molecular dynamics simulations, and found that densely packed semiflexible polymers cannot exhibit uniform nematic order when their contour length is of the same order as the sphere radius. Instead, the confinement leads to the emergence of topological defects on the sphere surface with competing ordering in the interior of the sphere. Each of the configuration variables including chain length, chain stiffness, packing density, and shell thickness uniquely affect the ordering, including the nature and relative orientation of the defects on the surface. For example, at high densities, a thin shell of polymers close to the surface exhibits a quadrupolar tennis ball texture due to the confinement-induced gradual bending of polymer bonds. Systemic trends observed could pave the way for better understanding the links between topological defects and elastic properties of polymers. Further, controlling the defect locations is promising for designing patterned colloids in experiments by functionalizing defect sites.

PO5 Development of coarse-grained models for polymer materials

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The use of generic coarse-grained (CG) model combined with mesoscopic methods has been successfully applied to reproduce universal properties of polymer melts in terms of scaling laws. However, when we want to consider the chemical nature of the monomers, we need to develop realistic CG models. Different strategies coexist : a top-down approach consisting in parameterizing the CG model from macroscopic properties and a bottom-up approach aiming to design the CG force-field from atomistic configurations. In the bottom-approach, the CG potentials can be obtained from methodologies based on the structure [1-3] and on the reproduction of the trajectory [4] at the atomistic scale. We use here a new Bayesian method which consists of optimizing the energy parameters of the CG model used in dissipative particle dynamics (DPD) simulations. We propose to discuss some fundamental aspect that may impact the performance of the CG model: i) the degree of coarse-graining, ii) the shape of the CG beads iii) the transferability of the model.

We will show recent results of different systems involving the interaction of polymer chains with silica surfaces and metal-oxide surfaces, in particular a model for cis-polybutadiene interacting with cuprous oxide. In addition, preliminary results for the crystallisation of polymers induced by shear and strain, and the mechanical properties of CG cross-linked networks will be presented.

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PO6 Deswelling effects on transport properties of ionic microgel suspensions

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Microgels are solvent-containing, cross-linked polymer networks of colloidal size that can reversibly swell or deswell in response to external stimuli. Ionic microgels, in particular, are highly sensitive to changes in environmental conditions such as temperature, solvent quality, polymer cross-linking, suspension ionic strength and particle concentration, which allows for controlling their size and effective interaction. In this work, we study theoretically the effects of concentration-dependent deswelling of weakly-crosslinked ionic microgels on dynamic and structural suspension properties [1]. We use and compare two different theoretical approaches to calculate the equilibrium microgel size, namely the Denton-Tang method based on a Poisson-Boltzmann cell model [2], and a multi-colloid center based thermodynamic perturbation method [3]. In combination with an effective interaction potential for spherical ionic microgels derived by Denton [4], we compute static pair correlation functions and structure factors. These are used as input in our calculations of dynamic suspension properties including the hydrodynamic function, collective diffusion coefficient, and high-frequency viscosity. As a consequence of the concentration-dependent deswelling, the collective diffusion of ionic microgels is enhanced while the suspension viscosity is lowered. We finally discuss charge-renormalization effects in ionic microgels.

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PO7 Coupled phase separation and surface migration in binary polymer gels: A multiscale simulation study

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When a mixture of polymers of differing molecular weights having a surface that is exposed to atmosphere is left to equilibrate the small molecular weight component migrates to the surface. A competition between loss of entropy and gain in surface energy determines the amount of material that migrates[1]. For well-mixed systems the concentration profile is near exponential with the oligomer concentration decreasing monotonically from the surface concentration to the bulk value as a function of depth. A macroscopic wetting layer forms for systems for which the bulk equilibrium thermodynamic phase is demixed. It has been shown recently that for systems for which one component is a gel the surface migration can be controlled by increasing the bulk modulus of the gel[2].

Moving beyond mean field calculations [2] we study the phenomenon of surface migration of oligomers in a polymer-oligomer mixture via coarse-grained molecular dynamics (MD) simulations and numerical solution of meso-scale hydrodynamics equations using Cahn-Hilliard-Cook (CHC) formalism, with the Flory-Huggins free energy functional describing the polymer-oligomer mixture. We find that domain length $\ell(t) \sim t^{1/3}$, following a Lifshitz-Slyozov scaling law and compute concentration profiles as a function of depth. As quenched polymer coarsens we measure tagged particle dynamics of oligomers. We find that the single molecule dynamics is dominated by fluctuations, and though the linear mean squared displacement implies Fickian dynamics, the Van-Hove function (VHF) and non-Gaussian parameter indicates non-Gaussianity. The exponential tails of VHF indicates existence of slow and fast modes signatures of glassy dynamics. System intrinsically not glassy but dynamics indicates heterogeneous dynamics. To the best of our knowledge signatures of glassy dynamics in phase-separating binaries have not been reported.

We report novel simulation results using both formalisms (CGMD, and CHC) that show that upon gelling one of the components, the surface migration of the oligomers is significantly reduced at long times. Gelation is further changes the coarsening exponent of $1/3$ corresponding to model B dynamics. Gelation induced in the MD simulations by introducing explicit bonds between nearby end-beads of the polymers and in the CHC formalism by incorporating a Flory-Rehner type term in the free energy.

This framework provides a multiscale approach to quantitatively predict the migrant fraction of oligomers in polymer-gel binary mixtures that relate physical parameters at the mesoscale to macroscale. Since small molecule migration leads to loss of function an understanding of the parameters that control surface migration is crucial for designing industrial products with well-tailored functional properties.

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PO8 Soft micron-sized hollow rods of high aspect ratio

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"Rod-shaped particles are ideal anisotropic systems for studying the isotropic-nematic-smectic phase transitions. Micron-sized silica rods have been extensively employed as model particles in the investigation of such colloidal phase transitions, because of their facile synthesis [1], which also enables their labelling with fluorescent dyes [2], and the ability to visualize them using an optical microscope. However, one of the main drawbacks of these particles is their high density (d $\sim$ 2 g/mL) which leads to fast sedimentation of the colloids in common solvents such as ethanol, water, etc, and renders the density matching of the system very challenging. In the present study, hollow polymer rods were synthesised by first growing an amphiphilic block copolymer brush from the surface of micron-sized silica rods, using surface-initiated atom transfer radical polymerization [3], followed by etching of the inorganic core with a concentrated hydrofluoric acid solution. The presence of the inner hydrophobic block was found to be crucial for the synthesis of the rod-like hollow particles, whereas the hydrophilic shell served as the stabilising layer in water, but could also be used to confer additional properties (i.e. responsive behaviour) to the hollow colloids. The influence of the size of the hydrophobic and hydrophilic blocks and the cross-linking of the inner polymer layer were exploited in the morphology, wall thickness, flexibility and the stability of the obtained hollow structures. Fluorescently-labelled rods were also obtained using a functional co-monomer during the growth of the brush. The rod assemblies in aqueous media were characterized by optical and fluorescence microscopy. The significantly lower density of the hollow polymer rods prepared herein, compared to their silica precursors, is highly advantageous in liquid crystalline phase behaviour studies.

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PO9 Self assembled linear polymeric chains with tuneable semiflexibility using isotropic interactions

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We propose a two-body spherically symmetric (isotropic) potential such that particles interacting by the potential self assemble into linear semiflexible polymeric chains without branching. By suitable control of the potential parameters we can control the persistence length of the polymer, and can even introduce a controlled number of branches. Thus we show how to achieve effective directional interactions starting from spherically symmetric potentials. The self assembled polymers have an exponential distribution of chain lengths akin to what is observed for worm-like micellar systems. On increasing particle density the polymeric chains self-organize to a ordered line-hexagonal phase where every chain is surrounded by six parallel chains, the transition is first order. On further increase in monomer density, the order is destroyed and we get a branched gel like phase.

This potential can be used to model semi-flexible equilibrium polymers with tunable semiflexibility and excluded volume. The use of the potential is computationally cheap and hence, can be used to simulate and probe *equilibrium polymers* dynamics with long chains. The potential also gives a plausible method of tuning colloidal interactions in experiments such that one can obtain self-assembling polymeric chains made up of colloids and probe polymer dynamics using an optical microscope. Further, we show how a modified potential leads to the observation of an intermediate nematic phase of self assembled chains in between the low density disordered phase and the line-ordered hexagonal phase.

1. Self Assembly of Linear Semiflexible polymeric chain using spherically symmetric potentials. Authors: Alex Abraham, Apratim Chatterji. J.Chem.Phys. **148**, 154901 (2018).

PO10 Exploiting Scaling Laws for Designing Polymeric Bottle Brushes: a Theoretical Coarse-Graining for Homopolymeric Branched Polymer

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Bottle brushes are polymeric macromolecules made of a linear polymeric backbone grafted with side chains. The choice of the grafting density σ_g, of the length n_s of the grafted side chains and their chemical nature, fully determines the properties of each macromolecule, such as its elasticity and its folding behaviour. Typically experimental bottle brushes are systems made of tens of thousands of monomeric units, rendering a computational approach extremely expensive, especially in the case of bottle brushes solutions. A proper coarse graining description of these macromolecules, thus appears essential.

We here present a theoretical approach able to develop a general, transferable and analytical multi-scale coarse graining of homopolymeric bottle brush polymers. Starting from scaling theories, each macromolecule is mapped onto a chain of tethered star polymers, whose effective potential is known from scaling predictions, computational and experimental validations and can be expressed as a function of the number of arms f, and on the length n_a of each arm. Stars are then tethered to one another and the effective potentials between them is shown to only depend on the key parameters of the original bottle brush polymer (σ_g, n_s). The generalised form of the effective potential is then used to reproduce properties of the macromolecules obtained both with scaling theories and with simulations. The general form of the effective potentials derived in the current study, allows to describe theoretically and computationally properties of homopolymeric bottle brush polymers for all grafting densities and all lengths of both backbone and grafted arms, opening the path for a manifold of applications.

PO11 Contact Aggregation and Bridging of Athermal Nanorod Dispersions -A Molecular Dynamics Study

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In polymer nanocomposites, the shape of the nanoparticle plays a crucial role in how itorganizes within the host polymer. Anisotropic nanoparticles such as cubes and tetrahedra have been shown to agglomerate and organize into multidimensional structures depending on the particle volume fraction and the adsorption strength of the polymer[1]. The effect of the nanorod geometry and the rod-polymer attraction strength on the miscibility within the polymer matrix was investigated using PRISM (Polymer Reference Interaction Site Model) theory[2]. Theoretical calculations have found that an attraction between particle and polymer favours the dispersion of nanorods, but at high attraction strengths bridging and tele-bridging of the nanorods with the polymer chains has been predicted. It is also observed that at very low attractions, the nanorods are phase separated and aggregated due to the entropy driven depletion attraction between nanoparticles. At moderate attractions, there exists a miscibility window that lies between the depletion driven phase boundary at low particle-polymer attraction and the bridging driven phase boundary at high particle-polymer attraction. Further, as the length of the nanorod increases, the width of the miscibility window decreases.

The present work is aimed at comparing and ascertaining the predictions of the theoretical work using molecular dynamics simulations. We present a spinodal phase diagram showing the depletion and bridging boundaries as a function of nanorod aspect ratio and particle-polymer interaction strength. Qualitatively, our simulations agree with theoretical predictions, but the location of the phase boundary is quantitatively different from that predicted by PRISM theory. Moreover, the theory predicts that even in the absence of attraction, only the nanorods of short length and spherical nanoparticles are miscible with the host polymer and long range repulsions are necessary for them to deplete from the polymer. Whereas the simulation results show that, in the absence of particle-polymer attraction both short and long nanorods are miscible with the polymer. Further, it is also shown that long range repulsions are responsible for the depletion of nanorods of all aspect ratios. The molecular dynamics simulations agree with the PRISM theory and Dissipative Particle Dynamics[3] calculations which show that the depletion boundary rises as the length of the nanorod is increased.

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PO12 Nanocomposites Drying : Structural and Mechanical Analysis

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Nanocomposites Drying : Structural and Mechanical Analysis Keywords : Nanocomposite, Polymer, Silica, Structure, Mechanical Analysis The dispersion of nanoscale inorganic fillers within a polymer matrix may potentially lead to a significant improvement of some of its mechanical properties. One of the methods used to prepare these nanocomposite materials relies on solvent evaporation. We chose a system based on a polymer, poly(methacrylic acid), silica nanoparticles and water. In this system, the polymer conformation can be tuned from compact coils to extended coils by changing the pH whereas the polymer-silica interactions are controlled using different surface modifications on silica nanoparticles. The purpose is to correlate the structural properties of the solid materials to their mechanical characterization. Solid nanocomposite materials were first prepared into a mold with free upper surface and under different controlled relative humidity (RH). The bigger the RH, the faster the speed of drying will be, which may lead to different structures, and so, different mechanical properties.

Structure of these materials were analyzed by Small Angle X-ray Scattering (SAXS) and gave us information about silica's organization. Very compact or fractal structure were obtained depending on the system parameters. Then, these materials were also mechanically characterized by two methods, Dynamic Mechanical Analysis (DMA) and Atomic Force Microscope (AFM). In this way, modulus from different scales were measured.

The results obtained should help understanding the impact of the charge initial organization on structural and mechanical behavior of the final nanocomposites.

PO13 Static and dynamics of entanglements in the lamellar phase of block copolymers

GARCIA, Nicols A. (Institut Laue-Langevin, Grenoble, France); BARRAT, Jean-Louis (Universit Grenoble Alpes, Liphy, CNRS, France)

A comprehensive understanding of the underlying physics in the viscoelastic behavior of polymers is of fundamental interest but also is relevant to consider their technological applications. It is well-known that the mechanical properties of polymers in melts and concentrated solutions depend fundamentally on the molecular weight of the chains. Indeed, the natural inability of the chains to cross each other comes into play when the chain-length increases inducing mobility constraints for them; thus the so-called entanglements appear. Nowadays, we know the entanglements are a universal aspect of the polymer physics which occur in any flexible polymer system if the chain is sufficiently long and the concentration is high enough.

Entanglements in homogenous systems in bulk conditions have been extensively studied through simulations and experiments, and some elegant theories provide the conceptual frameworks to interpret their behavior. Furthermore, similar studies were recently reported on inhomogeneous systems like confined environments: thin films, nanocylinders, etc. However little is known about those topological constraints on heterogeneous systems and multicomponent polymers such as block copolymers (BCPs), a fascinating system which in the proper conditions of temperature and composition tends to self-assembly in periodic nanopatterns of high technological interest. In this work, we use a novel coarse-graining for simulating entangled polymers in order to investigate the viscoelastic properties of BCPs when they segregate in a lamellar morphology. We have performed a thorough analysis to characterize the statics and dynamics of such a system.

We found the entanglements are not homogeneously distributed in space but instead adopt a distribution related to the underlying pattern as a direct consequence of the periodic location of the segregated domains. Moreover, the interface separating nearby domains induces a surface effect decreasing the density of entanglement locally, this effect seems to depend on the segregation regime, being more extended and notorious for sharp interfaces, i.e., in strong segregation. Regarding the dynamics, we found the entanglements play a crucial role in the kinetic pathway to the equilibrium of the self-assembly process and seem to favor the stability of the topological defects of the pattern, an undesired effect when their technological applications are considered.

PO14 Self-organization of networks formed by block copolymer stars

GARLEA, Ioana C. (University of Vienna); LIKOS, Christos N. (University of Vienna)

The study of star polymers is not only motivated by their industrial applications but also by the theoretical interest they present, as they constitute a bridge between colloids and polymeric chains. Structurally block copolymer stars (BCS) are composed of a number of polymeric chains which all have one end attached to a single central point, the outer ends of each chain being functionalized such that they can attach to each other. Provided that their density is high enough, BSCs self-assemble to form networks where the connecting points are aggregates of functionalized ends. Here, we investigate the formation of such networks using Molecular Dynamics simulation. We find that, depending on the strength of the interaction between the attractive ends, we can distinguish three different types of networks architecture exhibiting very distinctive properties. The organization of the stars within the network is very different from what we would expect from self-assembly at the level of one single star. As it is to be expected, the rheological properties of the observed types of networks are also different.

PO15 A Node Coupling Approach to Modelling Random Fibre Networks

HOUGHTON, Mark (University of Leeds); HEAD, David (University of Leeds); WALKLEY, Mark (University of Leeds)

Inspection of many biomaterials at the microscopic level reveals complex arrangements of individual biopolymers with seemingly random orientation and position. Deeper understanding of the mechanical properties of biopolymers at the network level can provide further insight into the rich and dynamic behaviour observed in cytoskeletons of mammalian cells, as well as various other biomaterials such as collagen and tissue scaffolds.

On the study of the collective behaviour of the mechanical properties of biopolymers, current three-dimensional models are divided into on-lattice and off-lattice approaches. When considering how two fibres should be connected, on-lattice models prove more convenient, but are arguably less representative to actual biomaterials. Off-lattice models can provide more realistic insight, but require an additional linking step due to the low probability of two randomly oriented fibres directly intersecting. In many current models, linking begins by considering a single point along each of the two given fibres. One approach is to consider equally spaced (mass) points along each fibre and identify the pair with shortest distance. Another approach is to find the minimum distance between the two fibres, where each end of this distance is a point on each fibre. From here, it should be decided how to link these pairs. It is possible to merge the pair into one unique point, such that each fibre is deformed and prestressed. Instead, many models choose to insert a new ?cross-linking? fibre, leaving each pair in their original position and allowing freely-hinged rotation about each end of the cross-linking fibre. Naturally, this linking should only occur in the case that two fibres are suitably close.

We present a Mikado based athermal model, for which we predict the stretching and bending behaviour of a random fibre network when it is fixed at one boundary and subjected to linear shear at the opposite boundary. In our model we first take the cross-linking fibre approach, inserting a new fibre between the two points of minimum distance of each fibre pair. We demonstrate the performance and limitations of this model for random 3D networks through simulations. We then consider an alternative node coupling scheme, without introducing cross-links, that allows nodes to retain their original positions and also retains the interaction between fibres. In practice this is achieved through independent contributions being added to a single location in the global Hessian matrix during assembly of the numerical system. One benefit of this approach is that we effectively reduce the complexity of the system by removing cross-linking fibres, but also constrain the node pair such that any resulting stress from the shear is applied uniformly across both nodes.

In this talk we will compare the effectiveness of both our cross-linking fibre approach and our coupled node approach. We will discuss the benefits and drawbacks of a coupled node model, presenting results that are benchmarked against fibre cross-linked networks.

PO16 Microfluidic-based polymeric foams as potential photonic structures

Ilham Maimouni (Ecole Supérieure de Physique et de Chimie Industrielles), RUSSO, Maria (Ecole Supérieure de Physique et de Chimie Industrielles); MORVARIDI, Maryam (Ecole Supérieure de Physique et de Chimie Industrielles); COSSY, Janine (Ecole Suprieure de Physique et de Chimie Industrielles); TABELING, Patrick (Ecole Supérieure de Physique et de Chimie Industrielles)

Through the past decades, polymeric foams have taken more and more place into our modern world and have been used in a myriad of applications such as insulation building materials, food industry and photo-catalysis thanks to their interesting structural properties. Recently, 2D foams have been investigated to be self-assembled materials exhibiting interesting photonic properties. In the present study, we aim at exploring the 3D foams case. In this perspective, microfluidic technologies are used to develop 3D, solid, highly monodisperse polymeric foams by packing air bubbles in aqueous solution containing a polymer. The bubbles are produced in a PDMS (Polydimethylsiloxane) microfluidic chip and directly assembled in a microfluidic channel giving birth to highly tunable 3D foam. Indeed, by varying fluid pressures, the foam composition and the polymerization process, we manage to sharply control bubbles production and thereby govern the structural properties of the obtained material: porosity, pores size, connectivity and polydispersity. Electromagnetic simulations are then performed to study wave propagation in such foams, looking up for the existence of a photonic band-gap and opening the way for a new technological application of soft matter sciences.

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PO17 Controlled self-aggregation of polymer-based nanoparticles employing shear flow and magnetic fields

KAHL, Gerhard (Institut für Theoretische Physik, TU Wien, Wiedner Hauptstrasse 8-10, A-1040 Vienna, Austria); TONEIAN, David (TU Wien), LIKOS, Christos N. (University of Vienna)

Star polymers are macromolecules that consist of a central core, attached to which are a number of linear polymer arms. Depending on the chemical composition of the polymers, the stars may take on varying conformations. For example, if the polymer arms are constructed such that the segments closer to the star's core are solvophilic, while the free ends are solvophobic, the solvophobic parts tend to aggregate into patches close to the star's near-spherical surface. In dense solutions, self-assembly not only occurs at the intra-star level, but depending on the mean number of patches, mechanically stable lattices of star polymers have been studied in computer simulations in the literature [1].

In this contribution, we rely not on solvophobicity to cause clustering in our star polymer simulations, but instead decorate the free ends of the polymer arms with super-paramagnetic dipole moments. As the magnitude of the interaction potential of two magnetic moments depends on the strength of the moment-inducing external magnetic field, this gives the (computer-)experimentalist fine-grained control over the formation and stability of columns of magnetic particles in a star polymer [2, 3].

By introducing a shear flow, where the solvent's local velocity is a linear function of the position along the gradient direction, we further break isotropy of the system. We demonstrate that the reduced symmetry makes the relative direction of the external magnetic field, in addition to its strength, an important parameter in determining the qualitative behavior of the star polymer. We discuss three archetypical scenarios – the magnetic field pointing along the orthogonal flow, gradient, and vorticity directions of the shear flow, respectively – and report qualitatively different behavior in each case. The latter case exhibits particularly distinguished behavior, e.g. in that the star polymer undergoes a net whole-body rotation dependent on the shear rate. We show that this phenomenon, as well as a range of shape and size descriptors, are in large parts controlled by the number of self-assembled magnetic columns, which in turn is a function of the external magnetic field. Other quantities, however, such as the orientational resistance, follow a universal power-law behavior that is shared by most polymeric systems, including non-magnetic ones.

We conclude by giving a short outlook on further research and possible applications, such as in microfluidic mixers with an efficiency controlled by easily manipulable external fields.

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PO18 Viscoelastic Properties of Rigid Star-Like Polymers

KING, David (University of Cambridge); DOI, Masao (Beihang University); EISER, Erika (University of Cambridge)

We aim to theoretically describe the viscoelastic behaviour of suspensions of general rigid star-like polymers. These are constructed from rigid Onsager rods and interact only via kinetic constraints below a certain concentration, above which the excluded volume interaction becomes important and a liquid crystal transition is known to occur (Frenkel 1991, Blaak & Mulder 1998).

We present a simple method for calculating the linear viscoelastic properties for dilute suspensions of these polymers and show that their shape can always be designed such that the elasticity vanishes. Meaning the suspension behaves like a dilute suspension of spheres despite the particles being anisotropic. This raises the important question of the origin of the elasticity of dilute suspensions of rigid rods. We answer this question by relating the elastic stress to the entropy change associated with the deformation of the kinetic constraints imposed on a particle by its surroundings. The concentration dependence of the elastic response to step strain of these suspensions in semi-dilute suspension is then determined by this method and is shown to produce results consistent with the well-known Doi & Edwards theory of rigid rods. This method adds more detail to the original theory and is easily extended to wire-frame particles of general shape. Our results are then compared to simulations and experimental data.

PO19 Tunable polymer-liquid crystalline mixtures: phase behaviour and surface migration

KOLLI, Hima Bindu (University of Sheffield); MUKHERJEE, Biswaroop (University of Sheffield); CHAKRABARTI, Buddhapriya (University of Sheffield)

The phase behaviour of polymer mixtures is well understood [1]. The same can be said about liquid crystals, extended objects, that break rotational symmetry and self-assemble to form a plethora of mesophases [2]. However the phase diagram of liquid-crystal and polymer mixtures has been less explored. An important parameter that dictates the conformation of a polymer is the ratio of its persistence length ξ to its contour length L. For $\xi/L \approx 1$ a rod like conformation is adopted while for $\xi/L << 1$ a flexible chain results. A system of polymers and oligomers with varying persistence and contour lengths thus allows for one to explore mixtures of (i) rods, (ii) polymers, and (iii) polymers and rods.

In this work we explore the phase behaviour and phase ordering kinetics of a mixture of rods and polymers having an exposed surface that preferentially attracts the short chain component as a competition between entropic penalty and gain in surface energy using coarse-grained molecular dynamics simulations and mesoscale hydrodynamics.

Depending on the composition and quench temperature the equilibrium conformations of long rigid polymers form nematic and smectic domains with the domain length (computed from the correlation function) $\ell(t) \sim\sim t^{\nu}$, where ν is the coarsening exponent. The short flexible polymers are thus stuck within a nematic (N) or smectic-A (S_A) phase which in turn dictates their surface migration characteristics, in particular the migrant fraction and thickness of wetting layer.

Our work provides an elucidation of the various physical processes and their associated time scales that play a key role in phase ordering and migration of small molecules (in bulk as well as to the surface) for polymer-mesogen mixtures where breakdown of rotational symmetry leads to rich dynamical behaviour[4]. We believe that our work provides a way by which surface migration of small molecules in formulated products that have internal order can be controlled.

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PO20 Structure and dynamics of ring and linear polymer blends

KRUTEVA, Margarita (Forschungszentrum Juelich); ALLGAIER, Jürgen (Forschungszentrum Juelich); RICHTER, Dieter (Forschungszentrum Juelich)

The absence of the chain ends in polymer rings results in a compact structure and dynamics distinctly different from most other polymer architectures: Slow lattice animal-like loop displacement are accompanied by fast relaxing subunits (loops) [1]. In blends of ring and linear polymers a tiny amount of linear chains may lead to dramatic changes in viscosity and diffusion properties [2]. Pulsed field gradient (PFG) NMR has proven to be an invaluable tool for monitoring molecular displacements in a range of length scales from below 100 nm up to tens of micrometers at the time scale from tens of milliseconds to a few seconds. Experiments addressing translational diffusion and rheological properties of ring polymers and blends of rings and linear chains using PFG-NMR demonstrate a relatively clear picture for small rings [3,4]. The most discussed effect is a threading of polymer rings by linear chains of the matrix resulting in a broad distribution of diffusion coefficients [5]. Here, we report a PFG NMR study of the translational mobility of poly(ethylene oxide) (PEO) rings and their blends with linear matrices of different compositions. Large rings in long linear matrices display at least two well separated different diffusion channels that were characterized as due to multiple threading and single threading events respectively [6,7]. Even though the diffusive channels with characteristic times in the millisecond range would be expected to interchange, a detailed analysis in terms of a two-state diffusion model allowing for state changes reveals that within the experimental sensitivity no such exchanges take place.

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PO21 Thermodyanmics of Supramolecular Polymers with Hydrogen Bonding Ends

LEE, Eunsang (Institute of Physics, Martin-Luther University Halle-Wittenberg); PAUL, Wolfgang (Martin-Luther University Halle-Wittenberg)

Rheological properties of supramolecular polymers (SMPs) depend on their equilibrium structure including the size, the number, and the topology of aggregates. Due to the complex interplay between chain stiffness, sticker interaction, polarity along a chain, and polymer conformational entropy, it is difficult to theoretically predict the structure of SMPs. In this work we investigate the thermodynamics of SMPs with H-bonding ends in a wide range of densities. Replica exchange stochastic approximation Monte Carlo simulations with a coarse-grained models for polyethylene and polybuthylene glycols are used. Our heterocomplementary SMP system includes the same concentration of two different molecules, each of which is functionalized by different H-bonding stickers at both ends. The functionality of the association varies depending on the chemical structure of the two stickers, which is described by our H-bond potential and parameters. Our simulation gives two transition lines with decreasing temperature. The one at high temperature is between morphologies of free polymers and linear aggregates. The other at low temperature defines a transition toward gel or micellar morphology depending on polymer concentration, which can be identified by branching of sticker association.

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PO22 Hydrodynamic Inflation of Ring Polymers under Shear

LIEBETREU, Maximilian (Faculty of Physics, University of Vienna); LIKOS, Christos N. (University of Vienna)

Multi-Particle Collision Dynamics enable the modeling of Hydrodynamic Interactions (HI), which can significantly alter the dynamics of fully-flexible, ring-shaped polymers. We report on a hydrodynamically-induced inflation scenario under shear, unique to ring-shaped plymers. We use the Kremer-Grest bead-spring model and couple it to Multi-Particle Collision Dynamics and the Lees-Edwards boundary conditions for shear. By analyzing the velocity profile of the solvent around the polymer, we are able to isolate the influence of deflection of solvent particles from the ring's horseshoe regions, which leads to a self-stabilization of the polymer at a certain alignment angle for certain shear rates. This self-induced stabilization is accompanied by a cessation of tumbling. At the same time, the ring swells significantly in the vorticity direction, and the horseshoe regions on the stretched and swollen ring experience only very minor fluctuations in this configuration. The stabilization itself depends both on Weissenberg number and contour length of the polymer.

The effect is exclusive to ring-shaped polymers under shear, and it stems from the interplay of hydrodynamic interactions and topology. Furthermore, the same effect can be observed for knotted ring polymers. A knotted section will remain strongly localized under shear and act as a kind of 'stabilization anchor' against tank-treading. On rare events, it may tank-tread from one horseshoe region to the other in a sudden burst of motion, but will otherwise remain near either horseshoe region. Above a certain contour length, knotted polymer rings behave very similar to unknotted ones of the same contour length. Smaller knotted rings can exhibit a range of different behaviors. We suggest strong shear could be used to reliably tighten knots on rings and streamline the behavior of a polymer melt.

PO23 Structural properties of mixtures of stars polymers and long chains

LOCATELLI, Emanuele (Faculty of Physics, University of Vienna); PARISI, Daniele (Institute of Electronic Structure and Laser, FORTH and Department of Materials Science and Technology, University of Crete); MEROLA, Maria (Institute of Electronic Structure and Laser, FORTH); TRUZZOLILLO Domenico (Laboratoire Charles Coulomb, UMR 5221 CNRS, Universit de Montpellier); GAUTHIER, Mario (Faculty of Science, University of Waterloo); LIKOS, Christos N. (Faculty of Physics, University of Vienna); VLASSOPOULOS, Dimitris (Institute of Electronic Structure and Laser, FORTH and Department of Materials Science and Technology, University of Crete)

"We employ a novel coarse-graining approach[6], to study star-chain mixtures[1-4], in the limit of long chains. The coarse-grained approach is based on the calculation of the effective interaction between a star polymer and a short chain of length N_c =10 at infinite dilution. A multi-blob-like approach is then employed to coarse-grain chains of arbitrary length N_c . We study mixtures of star polymer and linear chains in the protein limit, i.e. when $q = R_h^c/R_h^s$ >1 . We find that the addition of linear chains makes the star fluid more structured, confirming experimental observation obtained through rheological measurements.

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PO24 Theory of twist-bend nematic phases for banana-shaped molecules with axial chirality

MATSUYAMA Akihiko (Kyushu Institute of Technology)

We present a mean field theory to describe twist-bend nematic N_{TB} phases of banana-shaped liquid crystalline molecules with axial chirality. We first obtain a tensor order parameter for the banana-shaped liquid crystalline molecules as a function of the bend angle and four orientational order parameter, which describe uniaxial and biaxial nematic phases. Depending on the bend angle and the strength of an oblique twisting power of the banana-shaped molecules, we calculate phase diagrams on the temperature$-$bend angle plane and examine the uniaxial and biaxial N_{TB} phases and phase transitions.

PO25 Rheology and light scattering on locust bean gum solutions

O'CONNELL, Adam (University of Leeds); MATTSSON, Johan (University of Leeds); EVANS, Mike (University of Leeds)

Locust bean gum (LBG) is a naturally derived polysaccharide, found in the endosperm of seeds of the Carob tree. It is of industrial interest, due to its natural origins and strong thickening ability at low concentrations. It is widely used in the food industry, as well as in the pharmaceutical, cosmetics, and textiles industries. LBG solutions presents interesting phase behaviour e.g. demonstrating gelation upon long-term storage or freeze-thaw cycling. Moreover, its behaviour in the presence of co-solvents such as sugars or polyols and in the presence of other biopolymers is rich and of interest to a wide range of applications.

We here present a study of aqueous LBG solutions where the polymer concentration, temperature and addition of co-solvents was varied. Results from bulk rheology, microrheology and light scattering will be presented.

PO26 Monodisperse Liquid Crystal Droplets for Bio

Parinamipura M. Naveen Kumar (Parinamipura M. Naveen Kumar); Kamendra P. Sharma (IIT Bombay)

My poster will describe fabrication of monodisperse liquid crystal (LC) droplets with the help of microfluidics approach. The micron sized droplets can be sequestered with various types of enzyme-polymer bioconjugates without perturbing either the LC microstructure or enzyme function. Further, the defects on the surface of LC droplets can be used to position auxiliary components (polystyrene beads coated with catalytic Pt nanoparticles). The LC droplet sequestered enzymes coupled with the auxiliary component gives rise to a mobile platform that can drive cascade reaction at the LC/water interface.

PO27 Thermoresponsive Block Copolymer Grafted on Core-Shell Nanoparticles

ROMA, Elia (University of Rome ‘Roma TRE’); CORSI, Pietro (University of Rome ‘Roma Tre’); CAPONE, Barbara (University of Rome ‘Roma Tre’); BRUNI, Fabio (University of Rome ‘Roma Tre’); GASPERI, Tecla (University of Rome ‘Roma Tre’); SCHROFFENEGGER, Martina (University of Natural Resources and Life Sciences Vienna); ZIRBS, Ronald (University of Natural Resources and Life Sciences Vienna); REIMHULT, Erik (University of Natural Resources and Life Sciences Vienna)

Since 1966, when the poly(2-oxazolines) (POx) were discovered, they have undoubtedly been recognized as a polymer class with high synthetic versatility and good biocompatibility, giving access to highly functional and adaptable materials.[1] The poly(2-oxazolines) are prepared through cationic ring-opening polymerization (CROP), which allows for a simple control of the reaction condition, mainly due to the absence of undesired termination, and even possible chain transfers are suppressed. Furthermore, the large available number of monomers with different side chain modifications opens the path towards the fabrication of innovative smart materials having a manifold of applications. [2,3]

Taking into account such observations, we envisage the possibility of designing and synthesizing a block-copolymer featured by: (i) a polar side chain (Fragment A), able to trap organic and/or inorganic compounds (e.g. heavy metal in wastewater or active principles for drug delivery applications); (ii) a thermoresponsive scaffold (Fragment B), able to change the interaction with the media by tuning the temperature. Subsequently, we intend to graft these polymers onto iron oxide nanoparticles (high grafting density) or on organic cores.

Herein we report our results involving the synthesis of the two Fragments (A and B) and the consequent grafting system to the nanoparticles. Finally, we present the test for heavy metal binding in combination with the thermoresponsive behavior of our products.

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PO28 Connecting elasticity and effective interactions of microgels: the validity of the Hertzian model

ROVIGATTI, Lorenzo (Physics Department, Sapienza University of Rome); GNAN, Nicoletta (CNR-ISC); NINARELLO, Andrea (CNR-ISC); ZACCARELLI, Emanuela (CNR-ISC)

The bulk behaviour of colloidal suspensions depends crucially on the microscopic details of the particle-particle interaction[1]. For polymer-based building blocks, the interactions depend on a large number of parameters such as the particle microstructure, its composition and related physico-chemical properties (solvophobicity, charge density, etc.). Among the huge variety of available systems, stimuli-responsive microparticles built out of polymer networks, so-called microgels, have emerged as one of the most interesting class of soft particles, from both the theoretical and applicative standpoints[2].

Here we employ a recently-developed method[3] to generate and simulate realistic *in silico* microgels. We first look at the single-particle mechanics by calculating the elastic moduli in the small-deformations regime. We then use Umbrella Sampling and a generalised Widom insertion method to accurately estimate the two-body effective interaction.

We show for the first time that the Hertzian theory works well for large separations, and that in this regime the single-particle elastic moduli can predict the amplitude of V(r) for a wide range of network topologies[4]. However, for smaller separations microgels start to strongly interact and change their shape and V(r) deviates from the predicted Hertzian behaviour, affecting the bulk behaviour of the suspension[4].

This work establishes a clear link between the microscopic network properties and the resulting microgel-microgel interactions, paving the way for a deeper understanding of the bulk behaviour of microgel suspensions.

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PO29 Standing up and peeling off of nanosized shish-kebab structures formed in melt-spun HDPE and nylon6/clay nanohybrid fibres

Sager, Wiebke F. C. (Microstructure Research, Peter Gruenberg Institute, Forschungszentrum Juelich); Vad, Thomas (Institut fr Textiltechnik, RWTH Aachen University)

Shish-kebab structures are known to develop after cessation of flow from semicrystalline polymer melts and/or upon uniaxial drawing in the processing of polymer films and fibres. The pre-nucleating shish is commonly assumed to align with the flow direction inducing orthogonal crystallisation of kebab-forming folded chain lamellae. Here we combine results from transmission electron microscopy (TEM), wide angle X-ray diffraction (WAXD) and/or small angle X-ray scattering (SAXS) to follow the microstructural evolution of the fibres upon drawing. For the high density polyethylene (HDPE) fibres we evidence for the first time a horizontal alignment of the main part of the shish-kebab nanostructures and therewith a meridional crystallographic a-axis alignment at a moderate extrusion rate. A crystalline a-axis orientation has so far only been reported for helically twisted kebabs, whereby the a- and c- (chain direction) axes rotate around the b-axis (chain fold direction). In our case flat shish-kebabs align perpendicular to the flow direction due to a diverging extensional flow at the end of the spinneret as predicted by Trebbin et al [1]. Increasing winding speed induces, due to the unidirectional pulling on the surrounding polymer chains, a gradual azimuthal reorientation and finally an axial up-right standing of the shish-kebabs (axial and meridional c-axis alignment). Crystal dimensions and orientation distributions determined from an extended WAXD analysis are used to model the two-dimensional SAXS intensities. The structural evolution of the polyamide 6 (PA6)/clay nanohybrid fibres depends significantly on the amount of organically modified nanoplatelets (NCPs), that are exfoliated and axial aligned in the as-spun fibre. NCPs impede formation of shish-like γ PA6 crystallites occurring in the unmodified fibres, but induce crystallisation of folded chain γ PA6 lamellae on their aligning surface sites resulting in orthogonal growth perpendicular to the fibre axis and the formation of nanohyrid shish-kebab structures. Mechanical drawing causes delamination of the formed lamellae and shish nucleation in the bulk. This leads to an unprecedented microstructural transition from nanolamellar (kebab-like) to nanofibrillar (shish-like) structures, that is hold up with increasing NCP loadings. The total crystallinity can be described within the Avrami model by a 2D decompostion of the nanolamellae followed by bulk crystallisation of the nanofibrils. The morphological transition observed precedes the strain induced structural transformation from the γ to the α PA6 polymorph that is retarded in the equatorial plane in the NCP presence. The present findings have a strong impact on establishing structure-property relationships and in designing advanced materials with polymeric or nanohybrid shish-kebab structures.

[1] M. Trebbin et al., PNAS 2013, 110, 6706.

PO30 Folded alkane chains and the emergence of the lamellar crystal

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Primary, secondary and tertiary structures are concepts used to classify the structure formation of proteins in their native state. Chemical sequence (primary structure) gives rise to locally ordered chain segments (secondary structure) which arrange in a fixed three-dimensional pattern in the folded globular state of the protein (tertiary structure). Here we show by means of Stochastic approximation Monte Carlo simulations [1,2] that the same concepts can be applicable to synthetic polymers like polyethylene [3]. Although lacking primary structure and being simple homopolymers, short alkane chains fold into non-trivial ground states (tertiary structure) consisting of chain segments of defined secondary structures. These structures are defined by specific sequences of dihedral angles along the chain [4], similar to α-helices and β-sheets in proteins. The folded lamellar crystal typical for polyethylene chains requires a minimum chain length to occur as the ground state folded structure, which we identify to be around 150 repeat units [4]. The competition between chain stiffness and chain collapse underlies this complex structure formation.

[1] F. Liang, C. Liu, R. J. Carroll, J. Am. Stat. Assoc. 102, 305-320 (2007)

[2] T. Shakirov, Comput. Phys. Commun. 228, 38-43 (2018)

[3] W. Paul, D. Y. Yoon, G. D. Smith, J. Chem. Phys. 103, 1702-1709 (1995)

[4] T. Shakirov, W. Paul, J. Chem. Phys. 150 (2019)

PO31 Topological effects in cross linked bundles of semiflexible filaments

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Bundles of stiff filaments are ubiquitous in the living world, found both in the cytoskeleton and in the extracellular medium. These bundles are typically held together by smaller cross linking molecules. Some recent numerical studies of such cross linked semiflexible filament bundles as well as imaging of in vitro filament systems shows that bundles are can be kinked. They have localized regions of high curvature that appear to be at least long-lived metastable states. We propose that the observed kinks can be understood as the response of the bundle to local braid structures stabilized by the cross linking. We consider a simple model of such topologically protected braids related to instantons. Using that model we show that for sufficiently soft filaments or in the limit of sufficiently high cross-linker concentration the bundle locally bends to relax elastic energy near the instanton, producing a kink. We comment on the expected density of such kinks if they are equilibrium structures. Comparing that equilibrium density to those observed in experiment should provide insight into the kinetics of bundle self-assembly.

PO32 Dynamics of a polymer-nanoparticle composite: Effect of nanoparticle size and volume fraction

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Understanding the motion of nanoparticles in polymer solutions and melts is a problem of broad importance, with applications to many different fields, such as material science, biophysics, and medicine. If the nanoparticles are larger than the polymer's radius of gyration, their structure and dynamics can be well described in terms of effective pair potentials. However, much remains to be understood in the so-called 'protein limit', where the size of the nanoparticles becomes comparable to or smaller than that of the polymers. Moreover, most of the previous studies considering this size range have only focused on the dilute nanoparticle regime, which is easier to handle since inter-nanoparticle interaction can be neglected and the properties of the polymer solution/melt are expected to be unchanged.

Using molecular dynamics simulations, we study the structural and dynamic properties of a semidilute polymer solution containing well dispersed spherical nanoparticles of size smaller than the polymer's radius of gyration. We consider various nanoparticle diameters and a broad range of nanoparticle volume fractions, up to values for which the inter-nanoparticle interaction becomes important.

We find that the polymers slow down when the nanoparticle concentration is increased, in qualitative agreement with the confinement parameter theory [1], according to which polymers slow down because they have to squeeze through 'bottlenecks' created by the presence of the nanoparticles. We observe, however, that a purely geometric confinement parameter is not able to capture the dynamics of the polymers at lower temperature: we introduce therefore a (temperature dependent) dynamic confinement parameter, which allows to describe data at different temperatures using a single master curve [2].

Also the nanoparticles slow down when their concentration is increased, with the magnitude of the slowing down depending in a non-trivial way on their size. Surprisingly, if the concentration of the nanoparticles is increased past the range in which the nanoparticle dispersion is good, the diffusivities of both polymers and nanoparticles reach a minimum and then start to increase [2].

[1] Choi et al., ACS Macro Lett. 2013, 2, 485?490

[2] Sorichetti et al., Macromolecules 2018, 51, 5375?5391

PO33 Freedericksz transition in dual frequency nematic liquid crystal PCPB / MBBA mixtures

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Dual frequency nematic liquid crystals (DFNLCs) are liquid crystals that the sign of dielectric anisotropy varies depending on frequency of an applied electric field. At low frequencies, the dielectric anisotropy in PCPB / MBBA mixtures that we used is positive, while above the crossover frequency, that becomes negative. In general, orientational states between the vertical and horizontal orientations in liquid crystal devices are controlled by applying and removing the electric voltage. On the other hand, using the dual frequency liquid crystal, both orientations can be controlled by applying voltages with two frequencies higher and lower than the crossover frequency, and speed-up in the alignment control can be expected. We have already clarified the dielectric dispersion, the origin of dielectric anisotropy, and the relation between crossover frequency and relaxation frequency [1].

The change of the alignment state due to voltage occurs at a certain threshold voltage, and is called Freedericksz transition. Since the dielectric anisotropy depends on frequency of the electric field in the dual frequency liquid crystal, it is predicted that the threshold voltage depends on the frequency of the applied electric field. However, unfortunately, no frequency dependence of the threshold voltage in PCPB/MBBA mixtures has been examined yet, as far as the authors know. Under this circumstance, we investigated frequency dependence of the threshold voltage with respect to the Freedericksz transition in dual frequency liquid crystal PCPB / MBBA mixtures.

Liquid crystal mixtures were injected into the homogeneously and homeotropically aligned cells with a gap of 10 mm between the ITO electrodes. Observations of the Freedericksz transition were carried out with a polarization microscope. Changes in transmitted light intensity were recorded with a CCD camera, and threshold voltages were determined. It was found that the threshold voltage increases with approaching the crossover frequency, and diverges at that frequency. We confirmed that the absolute value of dielectric anisotropy is in proportion to the reciprocal of the square of the threshold voltage. These experimental results were found to be well explained by the usual theory for the Freedericksz transition.

[1] Y. Takikawa, K. Kaneko, S. Odani, I.-H. Lee, and M. Iwata: Jpn. J. Appl Phys. 57 11UB02 (2018).

PO34 Complex coacervation of food grade cationic surfactant Lauric Arginate with anionic algal polysaccharide Lambda Carrageenan

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Lauric Arginate Ester (LAE) is an approved food grade preservative that is cationic surfactant. It is a powerful anti bacterial and anti fungal agent. It is synthesised from three bio friendly components viz. Lauric acid, ethanol and arginine. In this study, we explore the underlying interactions, structure and foaming properties of cationic Lauric Arginate and anionic Lambda carrageenan complex coacervates.

Lauric Arginate interacts with carrageenan due to electrostatic interactions forming complexes[1]. It was observed that at low surfactant to carrageenan ratio they form soluble complexes, which are smaller than 50 nm in diameter. As the surfactant to carrageenan ratio was, increased formation of large insoluble complexes occurs leading to eventual phase separation of the system. Interestingly, with further increase in the surfactant concentration the complexes start to redispering in the water phase. This is due to the overcharging of complexes that makes them unstable and leads to dispersion. This is confirmed by particle size and zeta potential measurements.

The coacervation was observed to be significantly affected by addition of anionic surfactant Sodium dodecyl sulphate (SDS). LAE-SDS mixed micelles when mixed with carrageenan at different LAE/SDS ratio showed different extent of coacervation. While pure LAE-carrageenan mixtures show strong tendency to coacervation, addition of SDS indicated a sustained reduction in LAEs ability to form coacervates with carrageenan. This effect was due to formation of mixed micelles/vesicles of LAE-SDS which are more negatively charged than pure LAE micelles. At higher concentrations of SDS, the coacervate formation was totally suppressed, which is interesting. This was also confirmed by measuring heat of reactions using isothermal titration calorimetry. Structure of LAE-carrageenan complexes was also determined by Cryo-TEM and SAXS. It was observed that at LAE/Carrageenan ratio above 3 formation of lamellar complexes[2] was observed.

PO35 Microelasticity of deformable spherical diblock copolymer brushes

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Limited bonding valence is nowadays considered among the key ingredients to create complex structures with tailored properties; unfortunately, the synthesis of colloids with limited valence is often plagued by high polidispersity and non-scalability. These limitations can be overcome by employing molecular building blocks undergoing a hierarchical self-assembly process [1,2]. We consider a composite, star-shaped particle made of f diblock copolymer chains uniformly grafted on a spherical colloid. Each chain is composed by two kind of monomers: A-type monomers, in good solvent conditions, and B-type monomers, in bad solvent conditions. The latter are always located in the outer part of the particle and their interaction strength can be tuned. Depending on the relative abundance of B-type monomers and on the interaction strength, different chains may aggregate into clusters, that – following Capone et al. [3] – we name ‘patches’. We show that our system can self-assemble into a particle with a well-defined number of patches, similar to what observed for Telechelic Star Polymers [4]. In a successive step, we put the self-assembled, equilibrated particles under compression between two planar wall and we investigate how the confinement affects the elastic properties of our spherical brush as a function of the distance between the walls. We find that the number of these patches can be controlled by tuning the degree of confinement imposed to the particle.

[1] E. Bianchi, B. Capone, I. Coluzza, L. Rovigatti, and P. D. J. van Oostrum Phys.Chem. Chem.Phys., 2017,19,19847

[2] I. C. Garlea, E. Bianchi, B. Capone, L. Rovigatti, C. N. Likos Current Opinion in Colloid & Interface Science 30 (2017) 1-7

[3] B. Capone, I. Coluzza, F. Lo Verso, C. N. Likos, and R. Blaak, Physical Review Letters 109, 238301 (2012).

[4] L. Rovigatti, B. Capone and C. N. Likos Nanoscale, 2016, 8, 3288

PO36 Solid polymer electrolytes based on polymer blends

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Lithium ion batteries are important as power sources for many portable electrical devices (e.g. laptops and mobile phones) and the use of Li-ion batteries is predicted to grow substantially in the near future, whilst branching out into new application areas. Despite this rising demand, we presently lack safe, easy-to-process and thus low-cost, ideally mechanically flexible batteries. One way to achieve safe and flexible batteries is to use solvent-free polymeric electrolytes. However, a key challenge is to resolve how to decouple the ionic transport from the segmental relaxation and thus to achieve good transport properties combined with mechanical rigidity. Recent work has indicated the possibility of tuning the monomer structure in co-polymers to control the local packing properties, dynamics and ionic decoupling [1]. Another route is the use of polymer blends [2]. We will here present work that aims at a better understanding and control of the decoupling between ionic transport and polymer dynamics based on polymer blend based solid polymer electrolytes.

We present results for polymer blends based on ionically conducting polyethers (PPG) and more rigid, higher glass-transition polymers including polyalkyl methacrylates to which Li-ions are added. We present results from a wide range of experimental techniques including broadband dielectric spectroscopy (BDS), calorimetry, dynamic mechanical thermal analysis (DMTA), (cryo-) scanning electron microscopy (SEM/Cryo-SEM), small angle neutron scattering (SANS) and Atomic Force Microscopy (AFM). We present a systematic investigation of the ion transport, molecular dynamics and structure as well as rheology for a wide range of material compositions of these systems and discuss our results in the light of relevant previous literature and suggested models for ion conductivity and polymer blend behaviour.

PO37 The role of functionality on the branch point motion in star polymers

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Combining Neutron Spin Echo (NSE) spectroscopy and Molecular Dynamics (MD) simulations, the influence of the number of arms (functionality f) for different arm lengths on the branch point mobility in symmetric star polymers has been investigated [Holler et al., Macromolecules 51, 242 (2018)]. NSE experiments have been performed on centre labelled 3- and 4-arm polyethylene stars, which allow to directly observe the branch point motion on a molecular scale by measuring the dynamic structure factor. Large-scale MD simulations have been carried out for corresponding systems with f=3-5 giving access to much longer time scales. Both simulations and experiments reveal a stronger confinement for the branch point with increasing functionality. The dynamic structure factor has been analysed in terms of a modified version of the Vilgis-Bou model [Vilgis, Bou, J. Polym. Sci., Part B: Polym. Phys. 26, 2291 (1988)] for cross-linked networks. By incorporating dynamic tube dilution (DTD), where the tube parameters are renormalized with the tube survival probability (which is functionality independent), a good description of the NSE data and simulations for intermediate times was obtained. But the extended time range of the dynamic structure factor accessible by the simulations reveal a functionality dependent relaxation of the branch point which is not described by the DTD prediction.

PO38 PVdF-HFP/PVDF-based polymer blends and gels for Li-ion battery electrolyte applications

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Lithium ion batteries are important as power sources for many portable electrical devices (e.g. laptops and mobile phones) and the use of Li-ion batteries is predicted to grow substantially in the near future, whilst branching out into new application areas. Despite this rising demand, we presently lack safe and easy to process, polymer-based electrolytes with sufficient ion transport and mechanical strength for use in Li-ion batteries. One possible route is the use of polymer gels, where an ion-conducting non-polymeric fluid is combined with a polymer that contributes mechanical rigidity. Another route is to blend an ion-conducting polymer with a polymer which contributes the mechanical rigidity.

We here present results on both polymer blend and gel electrolytes based on either polyvinylidene difluoride (PVDF) or polyvinylidene difluoride-hexafluoropropylene (PVDF-HFP). The development of blend and gel ion transport, molecular structure, dynamics and mechanical properties will be discussed over a wide range of concentrations, temperature and salt conditions. Specifically, for the PVDF-HFP system, we have investigated polymer electrolyte blends made with poly(propylene glycol) (PPG) of varying molecular weight (134 2000 g/mol) to which plastic crystalline materials have been added to enhance the ion transport properties. Using this technique, we obtain good quality polymer blend membranes, characterised by elastic shear moduli of around 10 MPa and a room temperature ionic conductivity of up to 3×10^{-4} S/cm.

We present experimental results based on broadband dielectric spectroscopy (BDS), calorimetry, dynamic mechanical thermal analysis (DMTA), shear rheology, electrochemistry, (cryo-) scanning electron microscopy (SEM/Cryo-SEM), small angle neutron scattering (SANS) and small/wide angle X-ray scattering (SAXS/WAXS).

PO39 Magnetic properties of magnetoactive elastomers studying by molecular dynamics simulations

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Magnetic elastomers are the systems consisting of magnetic particles embedded in a nonmagnetic elastic matrix. We consider several models of magnetoactive elastomers. We use the Molecular Dynamics Simulations to study the different systems. The main interactions in systems under study are dipole-dipole magnetic one, Weeks-Chandler-Andersen potential, Zeeman energy, classical harmonic interaction. In order to introduce the elastic interactions we consider fixed nonmagnetic particles which are connected with dipolar or non-magnetic ones by springs. As the simplest model, we consider spherical magnetic particles in an elastic matrix. Also we take into account the shape anisotropy of magnetic particles. We can obtain the hysteresis loop of a magnetisation, radial distribution functions, etc. Also we can measure the First-Order Reversal Curves (FORCs) distribution, using a classical method [C. R. Pike et al., J. Appl. Phys. 85, 6660 (1999)].

PO40 Bioinspired structural color from phase separating polymers

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Structural colors are very common in nature, where they are produced by biological nanostructures able to provide a variation in the refractive index of a material on the order of the wavelengths of visible light. These structures can cancel, deflect or reinforce specific wavelength intervals, generating a permanent, very bright, non-fading color with no need of pigments or dyes. For example, in the feathers of certain birds the presence of phase-separated quasi-ordered structures generates non-iridescent blue colors [1]. Inspired by these, we aim to use phase separation to reproduce such colors in artificial materials, where biological components are replaced by synthetic polymers.

[1] E. Dufresne et al.; 2009; Soft Matter; 5(9), 1792-1795.

PO41 Quickly Reversible Structural Evolution Reinforces Slide-Ring Gels

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Conventional chemical gels are soft and elastic materials, but often show poor extensibility and mechanical strength due to the strong stress concentration at the shortest network strand resulted from the randomness of cross-linking reaction. To solve this problem, most of the reported tough gels introduce sacrificial structures which break at large deformations to consume strain energy input and relief stress concentration. However, large stress-strain hysteresis is unfavorable for many applications that require low stiffness, high strength, and quick response to deformation, such as sensors and actuators. Here we report a novel reinforcement strategy targeting soft, elastic and strong gels by introducing the movable cross-link junctions that are only topologically confined to the network without any strong bonding. We choose polyrotaxane (PR), a necklace-like supramolecular assembly with multiple ring-shaped α-cyclodextrins (α-CDs) threaded by axial polyethylene glycol (PEG), as the polymeric ingredient, and covalently connect the α-CDs in different PRs to fabricate so-called slide-ring (SR) gels. The network structure of a SR gel optimizes automatically by relative sliding movement between cross-links and polymer axes under stretching, resulting in the relieved stress concentration and further the remarkable extensibility. Moreover, such structural evolution is found to be quickly reversible so that SR gel retain pure elasticity. The axial PEG chains in SR network are so stretched that, as we increase the polymer concentration, the formation process of the strain-induced crystalline (SIC) structures is for the first time observed in hydrogel system. Due to the SIC behavior, SR gel not only exhibits the tensile strength of 1 MPa and the strain at break of more than 1300%, but also a slow fracture process with deviation and arborization at the crack tip. Our study provides a promising approach to enhancing the mechanical performance of the instinctively brittle polymer gels.

PR1 Rheology and extrusion 3D printing of nanocomposite hydrogels based on cellulose nanocrystals

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Hydrogels are hydrophilic materials that are capable to absorb large amounts of water without losing their structural integrity and are widely found in pharmaceutical, food and biomedical applications. In recent years, a rapid growth of novel applications of such systems in regenerative medicine and tissue engineering can be found. This is due to hydrogels high biocompatibility and hydrophilicity, providing an adequate environment for cell growth and proliferation, as well as adequate mechanical properties for soft tissue regeneration applications. Extrusion 3D printing is considered one of the main additive manufacturing methods for hydrogel scaffolds manufacturing. However, obtaining hydrogel scaffolds with adequate dimensional accuracy and controlled porosity is not a trivial task due to their complex rheological behavior, which is strongly affected by processing conditions. Also, in order to perform extrusion printing of hydrogels, they must have specific non-newtonian and viscoelastic properties that allow printability such as high shear thinning and solid-like linear viscoelastic behavior. In the present work, rheological properties and extrusion printing of nanocomposite hydrogels based on cellulose nanocrystals with alginate and carboximethylcellulose (CMC) were studied. The interactions of aqueous dispersions of CNC and polymer chains in appropriate compositions may result in printable gels for scaffolds manufacturing. The interplay between gel structure and rheological behavior were studied using dynamic light scattering, zeta potential and rheometry. Rheological properties such as steady-state viscosity, storage and loss moduli and thixotropy were studied aiming identifying adequacy for extrusion printing. The most suitable systems were used for printing scaffolds under different processing conditions and further crosslinked. The resulting scaffolds may have potential applications in tissue engineering.

PR2 Increasing the extensibility of chemically crosslinked hydrogels with dynamic coordination bonds

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Hydrogels are promising candidates for biomedical applications, such as targeted drug-delivery or tissue engineering. However, the intrinsic heterogeneity of the polymer network and the lack of dissipative mechanisms in the material makes them very fragile. In order to improve the mechanical properties of hydrogels, reversible physical crosslinks have been introduced into a chemically crosslinked network.

Inspired by the mussel byssus, an organ which allows mussels to attach to surfaces thanks to metal ligand coordination complexes[1,2], we developed a chemically crosslinked hydrogel of poly(acrylamide-co-vinylimidazole), physically crosslinked by metallic cation (Ni^{2+} or Zn^{2+}) – Imidazole coordination bonds. Those coordination bonds introduce a dissipation mechanism in the material, due to the reversible breaking and formation of the coordination bonds. The characteristic exchange time can be modified by simply changing the metallic cation used.

For each cation used we were able to determine the characteristic relaxation time of the dual crosslinked gels by rheological experiments, by studying the evolution of the storage and loss moduli over a characteristic frequency range. In tensile tests, we found the extensibility to be much higher for the dual-crosslinked gels than for the bare chemical gel (strain at break increases from 200% to 700%). The elastic modulus was found to increase with strain-rate, and, at fixed strain rate, to change with the metallic cation introduced: gels with Ni^{2+} ions had a higher modulus than gels with Zn^{2+} ions, that have a modulus close to the modulus of the chemical gel. The fracture energy of those gels is also modified in the same way by the addition of metallic cations: tensile tests realized on notched samples show that the energy needed to propagate a crack, and its propagation speed, both increase with strain-rate and are higher for gels with Ni^{2+} ions than for gels with Zn^{2+} ions.

In summary we introduced a simple method to create dynamic, dual crosslinked hydrogels, with increased extensibility, where dynamics and mechanical behavior can easily be controlled by changing the metallic cation introduced. The preparation method being quite versatile, a large variety of metallic cations can be used (such as, but not limited to, Ni^{2+}, Zn^{2+}, Cu^{2+} or Hg^{2+}). The elasticity of those gels is controlled by the number of active ('closed') physical bonds in the material: by increasing the strain-rate above the characteristic exchange frequency of the coordination bond, we increase the number of closed bonds and thus increase the elastic modulus of the material. By changing the metallic cation, we simply change the characteristic frequency of the coordination crosslinks, and thus shift the dynamics of the gel.

[1] Fullenkamp D.E., He L., Barrett D.G., Burghardt W.R., and Messersmith P.B., Macromolecules 46 (3): 1167-74, 2013. [2] Grindy S.C., Learsch R., Mozhdehi D., Cheng J., Barrett D.G., Guan Z., Messersmith P.B., and Holten-Andersen N., Nature Materials 14 (12): 1210, 2015.

PR3 Stressed magnetic droplets

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The shaping of small volumes of fluids has important applications in Droplet Microfluidics (DMF), where droplets are manipulated for mixing or sensing, and liquid lenses, where optical properties are determined by the shape of the fluid. Fluids can be shaped through the application of electromagnetic stress. Ions or electric and magnetic dipoles in the fluid experience a force in electromagnetic fields. The electromagnetic force on droplets can be calculated using the Maxwell Stress Tensor, which is a powerful tool derived from first principles of electromagnetism.

Electric stress on droplets dominates DMF literature. Previous work by T.B Jones and others has looked at an explicit evaluation of the Maxwell Stress Tensor surface integral for a limited set of well-defined problems such as electrowetting and dielectrophoresis [1]. Generally, the Maxwell Stress Tensor is not explicitly applied and evaluated, but leaps are made. Limitations of simplified equations are often not clearly stated, which causes the erroneous application of simplified models to related research questions.

Here, we explicitly apply the Maxwell Stress Tensor to para- and diamagnetic droplets in magnetic fields and calculate the electromagnetic force density as a function of the applied magnetic flux density. Our application of the Maxwell Stress Tensor extends previous work by Kang et al [2] to sessile para- and diamagnetic droplets and magnetic actuation. Starting from a full definition of the Maxwell Stress we systematically apply assumptions and simplifications for our research question. This transparent and easy-to-follow method applies previous work by Stierstadt and Liu [3] to magnetic DMF with small magnetic susceptibilities.

We test our force predictions by measuring the deformation of a paramagnetic droplet in a homogeneous magnetic field using a modified Young-Laplace equation. Our experimental deformation of paramagnetic droplets extends previous work by Mats et al [4] to a study of shape change as a function of susceptibility and volume of the droplet, and the magnetic flux density applied to the droplet.

To showcase the relevance of this study to DMF, we demonstrate lateral movement and mixing of magnetic droplets on superhydrophobic surfaces. We show that through careful consideration the Maxwell Stress Tensor can be simplified to give an intuitive understanding of the fundamental physics involved in the deformation and manipulation of droplets.

[1] Langmuir 2003, 19, 7646-7651

[2] Langmuir 2002, 18, 10318-10322

[3] Z. Angew. Math. Mech. 2015, 95, 4-37

[4] Anal. Chem. 2016, 88, 9486-9494

PR4 Fracture of diluted networks: cracking or yielding?

DUSSI, Simone (Wageningen University); TAUBER, Justin (Wageningen University) ; BURLA, Federica (AMOLF) ; KOENDERINK, Gijsje (AMOLF) ; VAN DER GUCHT, Jasper (Wageningen University)

Solids can break in fundamentally different ways. Brittle fracture occurs when a macroscopic crack suddenly nucleates and propagates throughout the material. Alternatively material can soften, due to damage accumulation, before reaching the maximum sustainable load and only then will break in a sudden fashion (quasi-brittle). Also yielding before breaking is possible: fracture occurs after the system has shown a maximum in the stress response (ductile failure). Finally, it might be even possible that a material would lose its rigidity in a continuous fashion, with diffuse damage that percolates the system. The 'when', 'where' and 'how' a material breaks are intimately related to its microscopic structure. However, in intrinsically disordered materials, such as soft networks, neither the identification of the weak spots nor the prediction of how damage will spread are obvious tasks.

Computational studies on fracture of disordered materials have mostly relied on lattice models based on a scalar version of linear elasticity, called random fuse models (RFMs). It was shown that depending on the amount of disorder in the threshold distribution, fracture can indeed range from percolation to crack nucleation. However, in spite of the disorder, crack nucleation is predicted to unavoidably occur in large systems [1]. Crucially, RFMs do not take into account material rigidity. On the other hand, recent studies [2,3,4] suggest that rigidity plays a key role in material failure, to the point that stress concentration (and therefore crack nucleation) could be even suppressed at all length-scales [3]. These claims were based on simulations of moderate system size [2,3] and fracture experiments on small meta-materials [2,4]. Nevertheless, these predictions might be of extraordinary relevance for collagen fibre networks, that display a biologically crucial strain-stiffening response, due to the underlying strain-driven rigidity transition caused by their sub-isostatic structure [5].

In this talk, I will first show results from extensive off-lattice simulations of diluted spring networks with different topologies, connectivity, thresholds, and unprecedentedly large system sizes. We observe that even in large sub-isostatic networks with small thresholds, fracture occurs via crack-nucleation in a quasi-brittle fashion, in contrast with previous predictions [3]. However, the main descriptors of fracture (e.g. number of broken bonds, material strength, peak strain) exhibit power-law scalings, differently from RFMs, that depend on rigidity-related properties, such as network connectivity. Surprisingly, the maximum stress drop displays non-monotonic behaviour, suggesting a crossing between different failure regimes upon increasing system size. Secondly, I will report results from fracture experiments conducted on fibre networks made of collagen extracted from different sources. By comparing experiments and simulations, we rationalize the fracture behaviour in terms of network connectivity and properties at the fibre level. These systematic experiments on truly large systems allow us to clearly assess the role of rigidity on material failure.

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PR5 Multiscale study of nonaffine dynamics in stressed soft solids at the yielding transition

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How the mechanical properties of soft amorphous solids connect to their intimate structure is an exciting area of research that presents interesting challenges to both theorists and experimentalists [1]. Amorphous solids, when deformed, present a deviation from affine displacement already in the linear regime, because of their heterogeneity. The non-affine displacement field plays a central role in setting both the linear and non-linear mechanical properties [2]. This is especially true for very heterogeneous and hierarchically structured materials, where several substructures, with different length scales, must be considered for modelling the response of the material to an external force. Here, we employ a modern experimental approach to study the microscopic dynamics of model soft solid samples. Our approach is based on observing the sample with a microscope during the imposition of controlled macroscopic shear deformation, both in the linear and in the non-linear regime. Video microscope movies acquired in these conditions are analysed with Digital Fourier Microscopy (DFM) [3] to extract the spatio-temporal correlation of the affine and non-affine dynamics. DFM analysis enables studying the shear-induced-dynamics simultaneously at various length scales, going from hundreds of nanometres to tens of microns. In particular a microscopic fluidization is observed during the yielding transition. Besides presenting the experimental results obtained with this method, we will also discuss the relationship of our approach with other scattering-based approaches, as well as with similar work [4].

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PR6 Flow-induced Structural Changes of Microemulsions studied by Microfluidic-SANS

FISCHER, Julian (Institute of Physical Chemistry, University Stuttgart); ADAMO, Marco (Imperial College London, Institut Laue-Langevin); RADULESCU, Aurel (FZ Juelich); PORCAR, Lionel (Institut Laue-Langevin); CABRAL, Joao T. (Imperial College London); SOTTMANN, Thomas (University of Stuttgart)

To investigate the structural changes of microemulsions under microfluidic processing, we utilize the newly developed microfluidic-SANS method. We fabricate a series of high neutron transmission microfluidic devices by closed-face frontal photopolymerization (FPP) to induce precise contraction-expansion flows with prescribed dimensions. Utilizing the extraordinary high scattering intensity of well-structured bicontinuous microemulsions, we choose the system comprising D_2O, *n*-octane and the linear non ionic surfactant tetraethylene glycol monodecyl ether ($C_{10}E_4$) for studying the flow-induced transition from bicontinuous to lamellar (L_α) structures at room temperature conditions (PIT = 23.0 C). The microfluidic devices impose an abrupt increase of the applied flow velocity by a factor higher than 20 across the flow constriction, which we deploy to induce a structural change of the initial bicontinuous microemulsion near the PIT with applied flow velocities up to 247 mm/s. Beginning with an initial flow velocity of 15.4 mm/s, we observe the emergence of an anisotropy which intensifies systematically with an increasing flow. By measurements in wider channels, at identical flow velocities, we are able to show that these structures do not result out of wall shearing effects inside the constriction. This structural change exhibits fast kinetics as it can be observed right from the beginning of the constricted channel and the bicontinuous structure reforms immediately when the channel widens again, in a quasi-steady state manner. Ongoing data analysis seeks to resolve whether the flow induces a coexistence of bicontinuous and lamellar structures, a deformed bicontinuous structure made of passage connected sheets of surfactant monolayers or a new, still unknown structure.

PR7 Time-dependent active microrheology in dilute colloidal suspensions

FRANOSCH, Thomas (Universität Innsbruck); LEITMANN, Sebastian (Universität Innsbruck); MANDAL, Suvendu (Universität Dsseldorf); FUCHS, Matthias (Universität Konstanz); PUERTAS, Antonio (University of Almeria)

In a microrheological set-up a single probe particle immersed in a complex fluid is exposed to a strong external force driving the system out of equilibrium. Here, we elaborate analytically the time-dependent response of a probe particle in a dilute suspension of Brownian particles to a large step-force, exact in first order of the density of the bath particles. The time-dependent drift velocity approaches its stationary state value exponentially fast for arbitrarily small driving in striking contrast to the power-law prediction of linear response encoded in the long-time tails of the velocity-autocorrelation function. We show that the stationary-state behavior depends nonanalytically on the driving force and connect this behavior to the persistent correlations in the equilibrium state. We argue that this relation holds generically. Furthermore, we elaborate that the fluctuations in the direction of the force display transient superdiffusive behavior.

Reference: Leitmann et al, Phys. Rev. Fluids **3**, 103301 (2018)

PR8 Entanglement effect in highly strained polymer melts

HSU, Hsiao-Ping (Max Planck Institute for Polymer Research, Mainz, Germany); KREMER, Kurt (Max Planck Institute for Polymer Research, Mainz, Germany)

Polymer melts undergoing large deformation by uniaxial elongation are studied by molecular dynamics simulations of bead-spring chains in melts. Applying a primitive path analysis to strongly deformed polymer melts, the role of topological constrains in highly entangled polymer melts is investigated and quantified in detail. We show that the over-all conformations of the primitive paths (PPs) of stretched chains follow affine deformation while the number and the distribution of entanglement points along the PPs do not. Right after deformation, PPs of chains retract in both directions parallel and perpendicular to the elongation. Upon further relaxation we observe a long-lived clustering of entanglement points. Together with the delayed relaxation time this leads to a metastable inhomogeneous distribution of topological constraints in the melts.

PR9 The effect of dispersion transport properties on the concentration-polarization layer in crossflow ultrafiltration

Park, Gun Woo (Institute of Complex Systems, ICS-3, Forschungszentrum Juelich); Brito, Mariano; Nägele, Gerhard

"Crossflow filtration is a pressure-driven separation and enrichment process for colloidal dispersions where the feed dispersion is continuously pumped through a membrane pipe. The transmembrane pressure (TMP) causes the solvent to flow out of the membrane, while the colloidal particles are retained inside the pipe. Consequently, a particles-enriched diffuse layer is formed near the membrane wall which reduces the filtration efficiency. This so-called concentration-polarization (CP) layer is due to the balance of flow advection of particles towards and gradient diffusion away from the membrane. In the ultrafiltration regime where Brownian motion dominates flow convection, the collective diffusion coefficient and the dispersion viscosity are the key transport properties determining the CP layer in conjunction with the TMP and transmembrane osmotic pressure. In this study, we present a finite-element (FEM) method for calculating the CP layer and suspension flow profiles in a crossflow ultrafiltration setup [1]. We show that the FEM-calculated CP layer profiles are in quantitative agreement with results obtained from a simplifying boundary layer analysis [1]. Results for the filtration and flow profiles are discussed for different globular dispersion particles including colloidal hard spheres (as a reference system), solvent-permeable particles such as non-ionic microgels [2], impermeable charge-stabilized particles [3], and ionic microgels with concentration-dependent size [4]. We pay particular attention to the effect of the different transport properties and osmotic pressure dependencies on the ultrafiltration profiles.

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[2] R. Roa et al., Ultrafiltration modeling of non-ionic microgels, Soft Matter 11, 4106-4122 (2015)

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PR10 Subdiffusion in soft crowded media

PETERSEN, Charlotte (University of Innsbruck); FRANOSCH, Thomas (University of Innsbruck)

Transport through complex crowded media is common in natural and industrially relevant systems. These include catalysts, ion-conductors, inside of cells, and in porous rock during oil recovery. Both experimentally, and in simple models, subdiffusive transport has been observed in heterogeneous crowded media. A theoretical explanation has been provided for the origin of this anomalous diffusion for the paradigmatic Lorentz model. In this simple model, a single particle moves with Newtonian dynamics through a random array of fixed spherical obstacles. The tracer particle has specular collisions with the obstacles. At the percolation point of the obstacles, the mean square displacement grows subdiffusively. We extend the Lorentz model towards realistic systems by replacing the hard-exclusion interaction with a soft repulsive interaction potential, and find that the system has a percolation transition dependent on the energy of the tracer particle. At this point the dynamics are subdiffusive.

PR11 Production of microfibers using solvent removal in microfluidics

PULLAGURA, Bhargav Krishna (Indian INstitute of Technology Bombay, Mumbai-400076,India); GUNDABALA,Venkata Ramana

Microfibers have become a topic of interest for many researchers due to their vast and growing applications in filtration, textiles, electronics, tissue engineering and in other fields of science and technology. Drawing, template synthesis, phase separation, self-assembly, wet spinning, electrospinning are common techniques for the production of microfibers. Microfluidic spinning techniques are recently developed and soon gained acceptance and acclamation of the research world. The major difference between conventional and microfluidic spinning technique is the control over the jet offered by microfluidics during the transition from liquid jet to solid fiber which enables to control the size of the fiber and can also assist to tailor the fiber with tuneable functionalities. Microfluidics techniques are also relatively cheap, easy to prototype and do not require extreme processing parameters. Co-flow, flow focusing are common flow geometries for the production of microfibers in microfluidics with photopolymerization and ionic crosslinking reactions as common solidification techniques.

We made a hybrid 3D microfluidic device with molded PDMS square channel and pulled cylindrical glass capillary with existing fabrication procedure to produce microfibers. The geometry is coaxial co-flow with complementary side flows. Solvent removal using the co-flowing liquid streams was used as solidification technique. Complementary side channels control the coiling of the fiber inside the microfluidic channel. Microfibers were produced and environmental scanning electron microscopy (ESEM) images showed that the fibers were smooth and homogeneous. We observed that the fiber diameter can be controlled by varying both the inner and outer flow rates. Control on the extent of coiling was also achieved and both highly coiled and single fiber were obtained using the same device.

PR12 Competing Time Scales Lead to Oscillations in Shear-Thickening Suspensions

RICHARDS, James (University of Edinburgh); ROYER, John (University of Edinburgh); LIEBCHEN, Benno (Heinrich Heine University Dsseldorf); GUY, Ben (University of Edinburgh); POON, Wilson (University of Edinburgh)

Suspensions are industrially ubiquitous. There exist mean-field models of their uniform, steady-state flow, but their spatio-temporally varying flows remain poorly understood. In the form of instabilities, such flows can be catastrophic in the processing of high-volume-fraction suspensions. Coupling suspension properties to those of the shearing system, we establish a time-dependent model. This is tested against observed oscillatory instabilities in two model systems, for which highly asymmetric shear-rate oscillations occur when the time scale for the formation of a frictional contact network is much shorter than the time scale for instrument acceleration. In the process, we measure the relaxation time of frictionally-jammed particles, not hitherto accessible to experiments. The coupling of fast contact network dynamics to a slower system variable should be generic to many other areas of high-volume-fraction suspension flow, with instrument inertia providing a paradigmatic example.

PR13 Synchronization of droplet breakup from oscillating interfaces of fluids

UM, Eujin (Ulsan National Institute of Science and Technology (UNIST)); Kim, Minjun (Ulsan National Institute of Science and Technology); JEONG, Joonwoo (Ulsan National Institute of Science and Technology)

Phase synchronization of oscillating objects can often be found in our surroundings, such as the pendulum clocks and metronomes mounted on the same structure [1, 2], and flagellar cells in a microscopic world [3]. Here we propose a droplet microfluidic platform as a novel experimental model system to investigate the fascinating phenomena of synchronization. We explored hydrodynamic interaction of two oscillating interfaces, using immiscible flows in a microfluidic channel. While the interfaces generate monodisperse microdroplets, to our surprises, we discovered an overlooked regime of synchronization in the droplet breakup sequence from each interface. The parameter space of channel dimensions, and the flow rates of immiscible fluids affecting the size and generation frequency of droplets was investigated, identifying regime of synchronization, a transition regime resembling beating of coupled oscillators, and also the regime of no interaction. We seek a quantitative way to determine each regime and a simple model to explain the emergence of phase synchronization between two oscillating interfaces. We believe the microfluidic system of droplet breakup provides a new avenue for understanding synchronization mediated by hydrodynamic interactions and viscoelastic properties of fluids. In the applications of using microfluidic droplets as microreactors containing various materials, our knowledge can be used to manipulate the sequence of microdroplet generation from multiple interfaces.

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PR14 Hydrodynamics and filtering of knotted ring polymers in nanochannels

WEISS, Lisa B. (University of Vienna); MARENDA, Mattia (University of Edinburgh); MICHELETTI Cristian (SISSA, International School of Advanced Studies); Likos, Christos N. (University of Vienna)

”Polymers exhibit a variety of topologies ranging from linear to cyclic and various knot types permanently captured on cyclic polymers, which are of importance in biology, rheology and material science [1,2]. Unfortunately, the lack of reliable topology-sensitive separation devices hinders a detailed understanding. Macromolecules of distinct topology consist of the same type and number of monomers, making it challenging to separate them using chemical approaches. Nevertheless, topology influences strongly their response to flow fields in concentrated [2] and dilute solutions [3,4].

Previously, successful separation strategies for linear and circular polymers have been developed [5], which unfortunately fail to separate knotted ring polymers from the unknot. Thus, we present a novel separation strategy employing spatially-modulated channels [6] taking hydrodynamic interactions via the Multi-particle collision dynamics into account [7]. Our results have a twofold implication. First, they provide a quantitative advancement of the topology-dependent mobility of rings in modulated channels, which was previously carried out without hydrodynamic effects [8]. Second, and more importantly, they bring a qualitatively new physical insight into the problem by exposing effects that are solely observable with the explicit treatment of hydrodynamic interactions. We show that we can not only separate the unknot from knotted structures, but as well polymers of distinct knot topology in a regime characterized by Peclet numbers smaller than unity. Furthermore, we observe two modes of translocation, where the knotted section either leads translocation or lags behind. The dominance of one mode over the other is determined by knot size, hydrodynamic effects and constriction radius, surprisingly the preferred mode does not impact the separation efficiency. By controlling the constriction size, the mode can be successfully controlled opening new routes towards single molecule experiments.

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PR15 Semidilute mixtures of circular and linear polymers - towards novel separation techniques

WEISS, Lisa B. (University of Vienna); LIKOS, Christos N. (University of Vienna); NIKOUBASHMAN, Arash (Johannes Gutenberg University Mainz)

”Linear polymers have been extensively studied in various concentration regimes, at rest and when exposed to a variety of flow fields. Recently, this interest extended to ring polymer solutions, focusing on melts and dilute solutions [1,2] . At rest, dilute rings show the same scaling behavior as chains, but out of equilibrium astonishing differences become apparent uniquely related to their topology [1,3], which can be exploited for topology sensitive separation [4]. Furthermore, entangled ring polymer solutions show both in equilibrium and when sheared a distinct behavior compared to their linear counter part [2,5]. However, the semi-dilute regime of pure ring polymers and topological mixtures is poorly investigated so far. Here, we simulate pure linear and ring polymer solutions and their mixtures around the overlap concentration at rest and under pressure driven flow. To correctly take into account hydrodynamic interactions, we employ the Multi-Particle Collision Dynamics algorithm [6]. Mixtures of linear and ring polymers show at any investigated concentration distinct segregation behavior offering a promising route towards novel separation techniques [7]. In particular, a pronounced propensity of the rings to focus towards the channel center with the linear chains populating the region close to the confining walls is observed and quantitatively analyzed.

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PR16 Sol-gel coexisting phase of polymer microgel triggers buckling without applying pressure

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Mechanical buckling is a ubiquitous phenomenon of elastic bodies like core?shell microgels. Although conventional theory predicts that sufficiently high pressure is the primary factor inducing the buckling of core?shell microgels [1], they often buckle spontaneously without applying pressure [2]. For example, spherical microgels prepared from emulsion polymerization often buckle spontaneously without applying pressure. This indicates that the inhomogeneous internal structure of microgels in the sol-gel coexisting phase plays an important role in the spontaneous buckling. However, how the sol-gel coexisting phase in elastic bodies causes the buckling is still elusive.

In this study, we aimed to elucidate the underlying mechanism by which the inhomogeneous internal structure of polymer gels in a sol-gel coexisting phase causes spontaneous buckling without applying pressure. For this purpose, we used core-shell microgels prepared from aqueous two-phase systems (ATPS) of polyethylene glycol (PEG) and gelatin confined within lipid droplets [3-4]. The gelatin/PEG system enabled us to regulate the sol-gel coexisting phase by changing the quenching rate, because both, phase separation with complete wetting of gelatin on the lipid membrane and gelation of the gelatin, proceed with a decrease in temperature.

We demonstrated that the interfacial tension between the gel phase of the shell and sol phase of the core is responsible for the spontaneous buckling of the core-shell microgels. Our theoretical analysis reveals that spontaneous buckling occurs due to the balance between the gel elasticity and interfacial tension when the characteristic length is comparable to the microgel size [5]. Our findings provide new insights into the mechanism by which the inhomogeneous internal structure of elastic bodies causes buckling during polymerization and phase separation.

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PR17 A microscale approach to yield stress materials: investigation of nonlinearity and yielding with an optofluidic micro-rheometer

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The relevance of soft materials for our daily life is strongly nested in their multiple length scales and rich mechanical behaviour, viscoelastic response and flow properties, which are also critical for their processing. Microstructural dynamics and yielding mechanisms can be directly elucidated by probing nonlinear rheological properties at the microscale and comparing them to the macroscopic behaviour. However, passive microrheology is intrinsically limited to the linear response, while established active microrheology techniques, based on optical or magnetic tweezers, are typically limited to forces of few tens of pN, which allow to explore nonlinear properties only in extremely soft materials [Chapman, PRL 113, 098303 (2014)], or require complex setups which limit their application [Rich, Soft Matter (2011)].

We demonstrate that a recently developed microrheology technique, based on a microfluidic chip and optical scattering forces acting on a microbead [Nava, Soft Matter 14,3288 (2018)], can be implemented for both creep and oscillatory experiments, easily reaching hundreds of pN and thus providing access to a wide range of nonlinear phenomena. The design consists of two counter-propagating infrared beams carried into a microchannel by two facing waveguides, realized by femtosecond laser fabrication in a glass substrate. The relative intensity of the two beams can be temporally tuned by a shutter, providing a step function, or by an integrated Mach-Zehnder optical modulator oscillating between 0.01 and 10 Hz.

We exploit the potential of the optofluidic micro-rheometer for the investigation of yield stress fluids, which behave as liquids or as solids depending on the applied stress. Their threshold values are typically well beyond the range of the linear response. The origin and conditions of such a transition still display several open issues, related to the stress distribution within the material and the role of linear elasticity, so that comparing macroscopic and microscopic experiments can provide additional information to fill the gap [Bonn, Rev.Mod.Phys. 89,035005 (2017)].

We perform microscale creep, linear and nonlinear oscillatory experiments on yield stress materials with different microstructure: Carbopol, a well-studied benchmark material based on swollen microgels; a colloidal fibre network in a surfactant background; a hydrogel based on the self-assembly of DNA. Furthermore, by seeding the samples with small, passive tracers, we investigate the strain field and how the extent of the fluidized region around the moving microsphere depends on the applied stress and the material properties [Holenberg, PRE 86,066301 (2012)]. Once the portion of perturbed material and the stress distribution are properly considered, we find good agreement between the microscale yield stress values and bulk rheology estimates.

SA1 Physicochemical Interactions of Imidazolium-based Ionic Liquids with Monoglyceride Lipids

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Ionic liquids (ILs) are fascinating materials that are becoming very popular among scientists working in various areas including biological sciences. ILs are highly promising solvents for an extensive range of compounds, and exhibit a great potential for becoming ‘green solvents’. However, when it comes to biological applications their biocompatibility is of utmost importance [1]. Lipids are among the first and most vital set of molecules with whom the ILs are anticipated to interact within the biological systems. The research in this direction is pretty scarce and lacks deeper understanding of the most critical concepts. Here, we investigate some crucial physicochemical interactions between representative ILs and selected lipid molecules, monoglycerides.

Lipids, being amphiphilic, self-assemble into various structures including lamellar and bicontinuous cubic phase, with and without hydration, respectively. Both of these lipid systems are known to mimic biological membranes [2]. We employed these ‘model membranes’ and (separately) mixed with a range of custom-produced and commercial ILs. The ILs for this study were chosen attentively to allow the systematic variation of their hydrophilicity and lypophilicity, for instance, as a function of the structure of the N,N’-imidazolium sidechains and the nature of the anions. The ILs that we prepared and characterised in-house exhibited substituents (on imidazolium nitrogen atoms) from two groups: alkyls (linear and branched C1-C4) and alkoxyalkyls of the varying steric bulk, whereas the selection of counter-anions constituted hydrophilic halides and hydrophobic non-coordinating anions (e.g. tetraphenylborate).

The solubility and phase behaviour (mixing/demixing) at various compositions and temperatures, chemical interactions and nanoscale morphologies were studied, correspondingly, using aesthetic, spectroscopic and scattering techniques. This work is an important addition to the research towards biological applications of ILs, especially when they are anticipated to react with biomembrane systems.

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SA2 Machine learning phases of matter and spatially varying order parameters

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Statistical Mechanics is inherently a matter of dimensionality reduction and feature extraction: it tries to extrapolate a macroscopic description of a system in terms of a small number of thermodynamic observables from the enormous amount of degrees of freedom (of the order of Avogadro's number $\sim 10^{23}$) that describe the complex and largely stochastic behaviour of its microscopic components. In a broad sense, we could say that statistical physics did big data analysis before big data.

In particular, one of the main challenges of Statistical Mechanics is the understanding in terms of microscopic laws and first principles of macroscopic phase transitions, in which a drastic change of the macroscopic properties of a system occurs in response to a tiny variation of its thermodynamic conditions. In 1937 Landau formulated a highly successful phenomenological theory [1] – later justified from first principles – in which he assumed that different phases of matter could be characterised and distinguished by a single thermodynamic observable, called order parameter, and that the transition between phases could be theoretically addressed by expanding the system?s free energy as a power series in the order parameter.

Although for some phase transitions an order parameter can be built from symmetry considerations and the heuristic knowledge of the physics driving the transition, the determination of an appropriate order parameter to build a Landau theory for a generic phase transition is all but trivial. However, if we think about it with an agnostic approach, this can be reduced to a problem of dimensionality reduction and feature extraction, in a way that projects the high-dimensional phase space onto a low-dimensional manifold that accounts for most of the difference between two phases of matter.

Intriguingly, this is one of the most common and relevant problems tackled by Machine Learning – one of the most influent disciplines of the recent decades – which provides a large amount of methods and tools to perform dimensionality reduction and feature extraction. Recently, some of these methods have been applied to the 2D Ising [2] and the 3D XY [3] lattice models, showing how Machine Learning techniques can be successfully applied to the determination of order parameters.

Here we use Principal Components Analysis (PCA), an unsupervised learning method for dimensionality reduction, to study various liquid crystal phase transitions (isotropic to nematic, isotropic to cholesteric, nematic to twist-bend nematic), showing how machine learning techniques can learn the relevant features of various liquid crystal phases without any supervision, and recover the relevant spatially varying order parameters from literature, with a direct connection to Landau theories, proposing a paradigm to study novel phase transitions of yet unknown order parameters via machine learning.

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SA3 Density Functional Theory for Systems with Competing Interactions

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The low-T part of the phase diagram in systems with competing interactions is correctly predicted by the known versions of the density functional theory (DFT). The high-T part obtained in DFT, however, does not agree with simulations even on the qualitative level. In this work a new version of the DFT is developed. The contribution to the grand thermodynamic potential associated with mesoscopic fluctuations is explicitly taken into account. The expression for this contribution is obtained by the methods known from the Brazovskii field theory. In addition, we develop a simplified version of the theory valid for weakly ordered phases, i.e. for the high-T part of the phase diagram. The simplified theory is verified by a comparison with the results of simulations for a particular version of the short-range attraction long-range repulsion (SALR) interaction potential. Except from the fact that in our theory the ordered phases are stable at lower T than in simulations, a good agreement for the high-T part of the phase diagram is obtained for the range of density that was considered in simulations. In addition, the equation of state is presented. Finally, the physical interpretation of the fluctuation-contribution to the grand potential is discussed.

SA4 Phase behaviour of mixtures of hard and penetrable particles

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Systems of penetrable particles interacting through bounded potentials have been found to form clusters of multiple overlapping particles [1]. These clusters crystallize at high densities. Depending upon the softness of the bounded potential, different types of phase behaviours have been predicted by theory [2] and simulations [3]. We have used Polymer Reference Interaction Site Model theory (PRISM theory) to study the structure and phase behaviour of systems consisting of both hard and penetrable particles. Hard and penetrable particle mixtures are studied using four different cases: (i) the bounded repulsive potential is used to model the cross interaction between hard and penetrable particle, (ii) the cross interaction between two different hard particles is modelled by bounded repulsive potential, (iii) the cross interaction between hard and penetrable particle is given by hard sphere potential, and (iv) the cross interaction between two different penetrable particles given by hard sphere potential. When the hard and penetrable particle cross interaction is governed by bounded repulsive potential, we predict macrophase separation at high and low fraction of hard particles in the mixture. At intermediate hard particle fraction the system exhibits microphase separation. In the second case, when two different hard particles interact through bounded repulsive potential, macrophase separation is predicted at the extreme compositions of the mixture; at other compositions microphase separation is observed in the system. In the microphase separated region, the length scales of self-assembly for hard and penetrable particles or two different hard particles decreases with increase in interaction strength of the bounded repulsive potential. However, in the other two cases when hard sphere potential governs the hard-penetrable particle interaction or the interaction between two different penetrable particles, only dispersed phase is observed irrespective of the system composition. The changes in structure and phase behaviour of the mixtures of hard and penetrable particles as a function of composition and cross interactions are further studied using molecular dynamic simulations.

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SA5 Nucleation of pseudo hard-spheres and dumbbells at moderate metastabilities: appearance of A15 Frank-Kasper phase at inte

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In this contribution we present results of crystal nucleation of repulsive hard-dumbbells from the sphere to the two tangent spheres limit at moderately high metastabilities obtained by brute-force molecular dynamics simulations. Nucleation rates are in good agreement with previous simulations of hard-spheres and dumbbells. Icosahedral structures formed by twinned face-centred-cubic tetrahedra sharing five-fold symmetry axes and icosahedral centers are often found in spheres and dumbbells with either small (L/σ =0.1 and 0.2) and large (L/σ=1) elongations. These structures are incompatible with long range crystalline order but are able to survive up to quite large sizes. On the contrary, at intermediate elongations (L/σ =0.3), corresponding roughly to the bond length of molecular nitrogen, the fluid crystallizes into three distinct solid structures, namely, a low density plastic crystal, an hexagonal close-packed plastic crystal (with the same structure as β-N_2), and an A15 Frank-Kasper phase (cP8 structure corresponding to δ-N_2). At the lower pressures studied the hexagonal close packed plastic crystal is the most stable phase, but at the higher pressures the stable phase is an orientationally ordered solid designated as CP1 that is never spontaneously formed in our crystallization simulations.

SA6 Two-dimensional complex tessellations beyond triangular symmetry by sequential assembly of soft colloids

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The formation of controlled self-assembled complex two-dimensional (2D) patterns of colloidal particles with symmetries other than the triangular one is an elusive task. This typically requires particles with specific geometries (e.g. cubes or octahedra) or with patchy surfaces exhibiting directional interactions, finely engineered depositions or post-treatments (e.g. uni- or bi-axial stretching of elastomeric substrates). A general strategy to assemble the same uniform spherical colloids in a broad range of complex 2D patterns in a simple way is still missing. Here, we demonstrate that the sequential deposition of two hexagonal monolayers of the same soft colloids (microgels), pre-self-assembled at a water-hexane interface at controlled area densities, enables the realization of a wide variety of tilings with local triangular, rhombic, hexagonal and dodecagonal symmetries and even displaying complex hexagonal superlattices. We explain the experimental observations by means of systematic molecular dynamics simulations using effective soft repulsive potentials experimentally extracted from compression isotherms. Finally, by targeting specific assembly conditions, we demonstrate that the desired patterns can be realized over macroscopic scales. These results delineate how the design of soft colloids and the introduction of sequential assemblies enable the creation of very rich structures of potential interest for bio-interfaces, optics and metasurfaces.

SA7 Coarse Grained Simulations of Amyloid-β in Alzheimer's Disease

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"The pathology of Alzheimer's disease is governed primarily by the β-amyloid(Aβ) and tau τ proteins[1]. Monomers of Aβ protein aggregate into large fibrillar species, which have been found on the brains of Alzheimer's patients and also older brains generally ? and there remains question about a direct correlation between the presence of fibrillar Aβ and the diagnosis of Alzheimer's[2]. It is believed that some oligomeric intermediate species is/are the candidate for neurotoxicity[3] and that the presence of Aβ fibrils may catalyze the production of such toxic species. A second protein, τ, is hypothesised to form fibrils which tangle when hyperphosphorylated, causing neruone cell death[4]. This is believed to be driven by the production of toxic Aβ structures.

We report a multiscale computational approach, creating a coarse grained model of an amyloid protein with structural properties specific to Aβ that allows us to understand protein misfolding processes in general and make quantitative predictions of the Aβ self-assembly into fibrillar aggregates and the formation of oligomeric structures[5].

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SA8 Controlling crystal growth soft hydrogels

GERBER, Dominic (ETH Zürich); DUFRESNE, Eric (ETH Zürich), STYLE Robert (ETH Zürich)

Nature has shown that it is possible to take a basic set of common materials, and combine them in a structured way to make novel materials with exceptional properties. Nacre is a classic example, where brittle calcium carbonate is used as the basis for an incredibly tough biocomposite. In order to mimic such materials, we ideally need a way to self-assemble crystals in a material with controlled shape, size, orientation and spatial distribution.

One option for achieving this goal is to use hydrogels as a matrix to template crystal growth. Here, we study this process by growing $CaCO_3$ crystals in a neutral, PEGDA hydrogel. We use light microscopy to observe the dynamics of crystal formation in a milli-fluidic cell. In particular, we study how material properties of the hydrogel – such as stiffness, fracture toughness and network concentration – affect the resulting crystal growth. Our results shed light on the dynamics of crystal growth and ripening, and we find that we can grow crystals surprisingly uniformly throughout bulk hydrogel samples, with a high level of control over their size and spatial distribution.

SA9 Biomimetic Polymeric Membranes

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Amphiphilic polymers, like lipids, are able to self-assemble to form bilayer structures. These structures are fluid and able to reconstitute membrane proteins. Polymeric membranes are increasingly replacing lipid membranes in biotechnological applications due to their greater mechanical stability and resistance to air exposure. However, little is known about the formation and properties of supported polymeric membranes. To address this, we use a combination of AFM, fluorescence microscopy and mechanical tests to study membrane patches, formed by fusing giant polymeric vesicles to glass and silicone substrates. We present some unique observations on the fluidity and morphology of supported polymeric membranes and how they respond to mechanical stretch.

SA10 When bigger is faster: how non-commensurability in particle size favors self-diffusion in smectics

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Brownian particles usually exhibit complex dynamics when embedded in crowded host environment such as liquid crystals, colloidal crystals, biological membranes, and polymer glasses [1-3]. The general believe is that long particles experience a larger effective friction in such environments than short particles. In this work, we challenge the validity of this conjecture, by studying the self-diffusion of long guest viral rods immersed in a lamellar phase of self-organized shorter viral rods [4]. By using biological engineering for getting monodisperse filamentous viruses of tunable sizes, the length of the guest particles has been chosen to be 1.3 × longer than the host one, i.e. to be non-commensurate with the typical length scale of the host phase. Counter-intuitively, and inversely to the isotropic and nematic phases, it turns out that the long non-commensurate guest rods exhibit a faster self-diffusion in the smectic phase than the short host ones [4]. Using fluorescence microscopy, this dynamic behavior is quantitatively determined by single particle tracking of both guest and host particles, allowing for the measurement of their anisotropic diffusion coefficients as well as the time dependence of their probability density functions. An interpretation of these results based on free volume arguments will be discussed.

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SA11 Self-assembly of all-DNA patchy rods

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Stiff double-stranded DNA (dsDNA) forms a series of multiple lyotropic liquid crystal (LC) phases in aqueous saline solutions at sufficiently high concentrations [1,2]. DNA rod-like molecules exhibit cholesteric and columnar mesophases. However, no smectic ordering has been observed in monodisperse dsDNA fragments [3]. The absence of such one-dimensional layered structure can be attributed to the attractive blunt-end stacking interactions, which are weak non-covalent attractions between the ends of two base-pair terminated dsDNA helices [4]. In this work, we test the hypothesis that suppression of blunt-ended DNA stacking interactions could prevent the formation of linear polydisperse aggregates, and therefore, favor the formation of such layered mesophase over the columnar phase. Hence, we engineer these end-stacking interactions at the molecular level by constructing stiff DNA duplexes, which are capped on one or both ends with short PolyT loops. Through a combined experimental (small-angle x-ray scattering experiments) and numerical (Monte Carlo simulations) study, we provide unambiguous evidence that monolayer and bilayer smectic-A type of LC phases are formed by these capped duplexes. The formation of such phases suggests that the intermolecular stacking interactions can be selectively and effectively screened. Our results offer evidence that blunt-end stacking interactions play a crucial role in DNA self-assembly. This allows us to identify general guidelines for the re-examination of the LC phase diagram of short duplex DNA fragments with contour length L below the persistence length Lp of dsDNA (Lp 50nm).

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SA12 In sillico fibrillogenesis of collagen mimetic molecules

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One of the most remarkable examples of self-assembly in living organisms is the formation of collagen architectures. Collagen molecules robustly self-assemble into fibrils of well defined morphologies, which are crucial for determination of cell phenotype, cell adhesion, and tissue regulation and signalling. Collagen assembly is also at the centre of scientific efforts to design functional biomimetic materials and platforms for cell and tissue engineering. However, the current understanding of physical processes that drive collagen assembly and determine its resulting morphologies is far from complete. Here we develop a coarse-grained computer model of collagen-mimetic molecules that is capable of fibrillogenesis with specific D-periodicity. With molecular dynamics simulations we map the self-assembly behaviour as a function of the molecular charge pattern, the ratio between electrostatic and hydrophobic interactions, molecule flexibility, and molecule concentration. We analyse the kinetics of self-assembly and the morphologies of the obtained fibrils and networks. Our results identify the molecular determinants behind collagen fibril and network morphologies, and outlay design rules for assembling biomimetic collagen-like structures.

SA13 Coarse-Grained Modelling of DNA Hydrogels

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DNA hydrogels are based on multi-valent DNA structures with specific nucleotide sequences. They emerged as a distinct class of DNA material and attracted considerable attention due to their uses in controlled drug delivery, tissue engineering, for 3D cell cultures, cell transplant therapy and other biomedical applications.

Like in other examples of DNA nanotechnology, DNA hydrogels use the hybridization of single-stranded DNA into double-stranded DNA duplexes to design self-assembling, reversible structures with specific target shapes and connectivity, so-called DNA motifs. These motifs emerge when the DNA backbone is reciprocally exchanged between different duplexes. The Holliday junction, which plays a key role in meiosis, genetic recombination and DNA repair, is a well-know example that is based on the same principle.

I will present recent work on the melting behaviour, morphology and hybridized conformation of the building blocks of a previously introduced three-valent DNA hydrogel system [1] where the individual Y-shaped DNA molecules hybridize via sticky ends to form the percolating network structure. The overall aim is to gain a deeper understanding how the sequence may influence local structural features that can have a determining effect on larger length scales. The work uses the oxDNA2 model for coarse-grained simulation of DNA and RNA [2,3], which has been recently ported into the popular LAMMPS code [4] and is now amongst other LAMMPS-based CG DNA models.

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SA14 Stable structures of paramagnetic particles in precessing magnetic field

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Paramagnetic particles magnetizes in external magnetic field. Magnetization of the particle depends on external magnetic field and particle anisotropy axis direction. If such particles is exposed to stationary field they form chains, but if these particles is exposed to rotating field they form planes of particles. If we combine these two fields, we obtain precessing field which consists of stationary field which is perpendicular to rotation plane of rotating field. In this research it is found how structures (chain or plane) depend on precessing field parameters. Results are obtained theoretically and numerically. This talk will give insight how theoretical and numerical results are obtained and will show when you would obtain chain and when plane of particles in precessing field.

It will be taken into account that particles can be in synchronous or asynchronous regime depending on field parameters. For specific field parameters particles can form chains which form plane.

SA15 Electric Field Induced Self-Assembly of Highly Crosslinked Ionic Microgels: Correlations from Microscopic and Scattering Studies

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Electric field induced assembly is an attractive route to create fascinating three-dimensional structures within a short time scale. Ionic microgels of poly(N-isopropylacrylamide)-co-acrylic acid (PNIPAM-co-AAc) are ideal model systems to probe the structural ordering under an applied field, where numerous parameters can be tailored around such as the field strength, number of charges, cross-link density, number density, temperature, and pH. In ionic microgels with 5 mol% cross-link density, fluid, ordered and amorphous solid phases as a function of effective volume fraction and field strength [1] have been observed. These experiments provided evidence for a novel field-induced phase transition scenario with multiple path-dependent routes for phase-transition kinetics, and the existence of long lived metastable crystal states that were thought to be due to the ability of these particles to partially interpenetrate and form long-lived entangled states [1,2]. Here we make use of ionic microgels of higher cross-link density (10 mol%) in order to investigate the role of particle softness on the resulting field-induced state diagram. At low particle concentrations and at low field strengths (at a given frequency of 100kHz), the microgels assemble to form a fluid string phase. As the field strength is further increased, the particles assemble into small islands of body-centered tetragonal (BCT) crystals co-existing with a gas phase. These results are consistent with the field measurements on moderately crosslinked microgels [1,2]. At higher field strengths, however, the BCT sheets fold and adopt a regular tubular structure reminiscent of a single-walled microtubule. While ellipsoidal particles (polystyrene core, PNIPAM-co-AAc shell) polarized in an external electric field were observed to associate into well-defined tubular structures [4], no comparable self-assembly processes have been reported for hard or soft spherical particles so far. Given the intermediate degree of softness of the particles, we believe that this unusual self-assembly pattern is driven by a field-induced particle anisotropy. Here we present the results from a systematic investigation of the field-induced self-assembly of ionic microgels as a function of particle number density and field strength investigated through confocal microscopy, and correlate these results with the results from small angle neutron scattering (SANS) and small angle X-ray scattering (SAXS) studies. We discuss the underlying phase transition kinetics and plausible pathways for the various liquid-solid and solid-solid transitions present.

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SA16 Self-Assembling Block Copolymers in the Nucleation of Hydroxyapatite

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In the UK, tooth decay is prevalent in young children and tooth extractions are one of the top causes of hospitalisation of people under 18. The acidity in the modern-day diet causes increased dissolution of hydroxyapatite (HAP), which makes up 96% w/w of tooth. Saliva has a limited natural ability to protect enamel from demineralisation therefore an external remineralisation strategy is becoming an essential requirement for everyday life. The use of fluoride toothpastes have shown to repair damaged HAP with fluoride to form a mineral named fluoroapatite. However this can result in dental fluorosis which can lead to further health complications.

To address these issues polymers are under investigation for their effects on enamel. It has been theorised that having a self-assembled structure such as cylinders would allow controlled and directional HAP growth. This could be key to artificially synthesising morphologies that closely mimic natural enamel. Previously phosphorous-containing block copolymers have been reported to bind to enamel (HAP) and reduce the effects of acid erosion. However the effect of a self-assembled polymer on the growth of HAP has not yet been studied. The aim of this project is to design and synthesise self-assembling phosphorus containing polymers that bind to enamel. Through the secondary structure, the controlled nucleation and growth of HAP to facilitate the regeneration of lesions, or prevent demineralisation is to be investigated. Here di- and tri-block PEG based block copolymers have been synthesised through reversible addition fragmentation chain-transfer polymerisations in order to influence the nucleation of HAP. Through scanning electron microscopy, it can be seen that above the critical micelle concentration of the block copolymer the formation of calcium phosphate is promoted. The next steps is to use cryo-transition electron microscopy alongside electron diffraction to provide a time resolved study of the polymer's effect on HAP nucleation.

SA17 Novel hybrid crystal-liquid phase formed by heterogeneously decorated colloidal particles

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The self-assembly of colloidal particles is a very promising and adequate route to designed materials production that combines high flexibility, cost effectiveness, and the opportunity to create ordered structures at length scales ranging from nano- to micrometers. For many practical applications in electronics, photovoltaics, and biomimetic material synthesis, ordered layered structures are often urgently needed, as such lamellar particle arrangements stand out for their exceptional mechanical and optical features.

In this contribution it is demonstrated that charged colloidal particles with oppositely charged surface regions (so-called inverse patchy particles [1]) possess the unusual ability to spontaneously self-assemble into different morphologies of (semi-)ordered, layered particle arrangements, as has been witnessed in (quasi-)two dimensional geometries [2, 3]. The emergence of these patterns can easily be triggered, for instance, by the pH-value of the solution and/or by an externally applied electric field. In particular these particle arrangements are able to maintain their structural stability over a surprisingly large temperature range.

In three dimensions the capacity of these particles to form lamellar structures is based on the characteristic bonding pattern that these particles form via their oppositely charged surface regions: stable intra-layer bonds guarantee the formation of planar aggregates, while strong inter-layer bonds favour the stacking of the emerging planar assemblies. These two types of bonds are responsible for the remarkable self-healing properties that support the spontaneous self-assembly of these particles. Phases that emerge at low temperatures are characterized by highly stable parallel particle layers, strongly connected by a relatively small number of intra-layer particles [4]. While at low temperatures these phases are completely ordered, we observe that with increasing temperature a melting process of the inter-layer particles sets in: these particles become mobile and thus form a fluid phase, as witnessed by dynamical correlation functions. This scenario corresponds to a novel hybrid crystal-liquid phase, where a temperature-triggered transport process of the intercalated particles through an otherwise rigid structure becomes possible.

We provide via the phase diagram an insight in which density- and temperature range these lamellar phases are stable and give evidence where the different melting processes set in. In the high-density cubic phase we recover well-known two-dimensional positional and orientational patterns, which were identified in previous studies [2, 3].

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SA18 Opening and closing of particle shells on droplets via electric fields and its applications

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Active, tunable and reversible opening and closing of particle shells on droplets may facilitate chemical reactions in droplets and enable various small-scale laboratory operations, including online detection, measurement, and adjustment of droplet liquid. Manipulating various types of particle shells in a controlled manner requires new routes. This work provides a new strategy for controlling the spatial arrangement of particle-covered oil droplets using electric fields that expands the applica-tion of responsive droplet beyond the abovementioned examples. The behavior of stimulated particle-covered droplets is exploited in multiple ways: to form an active smart device; to produce new functional materials; to create an online diagnos-tic tool; and to produce a tool for fundamental studies. Electric fields are used to manipulate particle films on oil droplets through the synergetic action of droplet deformation and electrohydrodynamic liquid flows. First, the effects of electric field strength and liquid viscosity on droplet deformation, surface particle arrangements, and dynamics are examined in detail. Then, four examples of applications of responsive particle-covered droplets are demonstrated. Our results show that the reversible opening and closing of the droplet's shells, composed of various types of particles, can be conveniently achieved through electric fields, opening up a new possibility for applications in optics, clinical diagnostics, and material engineering.

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SA19 Pathways of amyloid aggregation on lipid membranes

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Amyloid aggregation is at the core of the two most common neurodegenerative diseases, Alzheimer's disease and Parkinson's disease. In both cases, soluble proteins assemble into abnormal fibrillar structures exhibiting high content of β-sheets consisting of Aβ42 and α-synuclein proteins, respectively.

Recent experimental findings have suggested that the interplay between cellular membranes and amyloidogenic proteins has a pivotal role in the assembly process of amyloid fibrils. In particular, the presence of lipid bilayers can dramatically speed up the the fibrillation of both Aβ42 and α-synuclein by enhancing the heterogeneous primary nucleation pathway. Specifically, the composition of the lipid membranes and their fluidity have experimentally been determined to play a crucial role in the propensity to form amyloids. Nevertheless, the precise mechanism by which lipid membrane control the nucleation and formation of amyloid fibrils remains poorly understood.

Here we develop a coarse-grained computer model to systematically explore the relationship between structural properties of the lipid membrane, the membrane affinities of proteins, and nucleation rates of fibrils. We find that both membrane fluidity and the membrane-protein affinity control the kinetics of amyloid aggregation. In fact, the fluidity of the lipid bilayer dictates to what extent the membrane participates in the amyloid nucleus formation thereby determining the nucleation kinetics.

SA20 Observation of Nematic Liquid Crystal Textures in a Fourier Phase Contrast Microscopy

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Phase contrast microscope is widely used in teaching and research labs to view transparent specimens, such as live cell cultures, which enables the study of dynamic biological processes. In the past we have developed Fourier phase contrast microscopy technique using photo-induced birefringence in liquid crystals that constitute a fascinating class of matter characterized by the counterintuitive combination of fluidity and long-range order. High power laser is passed through an optical microscope to facilitate the Fourier plane at the output of the video port. When the liquid crystal cell is placed at the Fourier plane, low spatial frequencies at the center of the Fourier spectrum are intense enough to transform local liquid crystal molecules into isotropic phase whereas high spatial frequencies are not intense enough and remain in the anisotropic phase. This result in a $\pi/2$ phase difference between high and low spatial frequencies, a basic requirement for phase contrast imaging. Liquid crystal materials are known for their exceptionally successful applications in displays, smart windows, and bio-sensing applications. Here we exploit different textures of a self-adaptive, nematic liquid crystal 5CB: planar, perpendicular, hybrid and twisted, and investigate their abilities to improve the contrast of phase images.

SA21 Heterogeneous local order in soft matter systems studied by X ray cross correlation methods

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Accessing structure beyond pair correlation functions is expected to shed light on various open questions in condensed matter physics such as the glass transition phenomenon and self-assembly processes. These phenomena are governed by the appearance of dynamical heterogeneities, suggested to be closely connected to spatial heterogeneities and believed to play a key role in the glass transition process. In order to measure such structural heterogeneities in scattering experiments, higher-order correlation functions have to be defined using e.g. the X-ray Cross Correlation Analysis (XCCA) technique.

Here, we will discuss our recent XCCA results on colloidal films and crystals [1,2]. A special focus is set on the structure of self-assembled films of gold nanoparticles coated with a soft poly(ethylene glycol)-based shell [3]. Depending on the initial concentration of gold nanoparticles, structurally heterogeneous films are formed with dominating four- and six-folds symmetry. The ordered domains have patch sizes of few micrometers whereby six-fold ordered domains are typically larger than others. Upon ligand modification of the gold particles as well as salt addition to the dispersion we find complex symmetry-selective order formation. This richness of information goes beyond two dimensional characterization and cannot be achieved by standard microscopy techniques that are commonly used to characterize such nanoscale systems.

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SA22 The effect of architecture and topology on the self-assembly of polymer-grafted nanoparticles

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Polymer grafted nanoparticles show a wide range of self-assembled structures in polymer melt [1]. In mixtures of polymers and nanoparticles, an entropy-induced depletion phase separation is observed. Recently, Tripathy [2] has done a study of polymer-linked nanoparticles where both ends of a chain are attached to nanoparticles. A chemically isotropic system was considered in order to isolate the effect of shape on the phase behavior. The system was found to self-assemble into alternating polymer-rich and nanoparticle-rich domains even for a chemically uniform system. In this work, we explore the effect of the architecture and topology of grafted-nanoparticle species on their phase behavior. Using Polymer Reference Interaction Site Model (PRISM) theory [3], we study three different architectures of such chemically isotropic species: singly grafted nanoparticles, doubly grafted nanoparticles and ring-grafted nanoparticles. The structure and phase behavior of these systems are studied as a function of the nanoparticle size and polymer length. We compared these systems with the polymer-linked nanoparticle system [2]. An anisotropic shape driven self-assembly is predicted for all these systems. The variation of the phase boundary (between the fluid and the self-assembled state) depends on both the polymer radius of gyration and the nanoparticle size. The transition from liquid phase to microphase separated structures is inhibited as the ratio of the nanoparticle diameter to the radius of gyration (D/Rg) value increases and the transition packing fraction attains a unique value at a certain D/Rg. This behavior is predicted for all the systems, irrespective of architecture and topology. We predict a weak dependence of microphase transition boundaries on the architecture and the topology of the polymer grafted nanoparticle systems. For these systems, the length scale of the self-assembly is a function of the fraction of the space occupied by the polymer and shows a universal scaling behavior. The singly grafted, double grafted and polymer-linked nanoparticle species follow the same scaling law as given for the polymer-linked nanoparticle species [2], while ring grafted nanoparticles follow a different scaling law, suggesting a strong dependence of the topology of the polymer grafted nanoparticles on the scaling behavior.

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SA23 Real-space study of homogeneous crystallization of (nearly) hard sphere colloids by arresting the dispersion

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The real-space study of colloidal crystallization on a single-particle level is only possible in a limited sample volume ($\sim$ 4000 particles), which makes it difficult to obtain large enough data statistics for investigating dynamical processes like nucleation and growth. We overcome this limitation by immobilizing the system locally on a time scale of 0.1 s by polymerizing a solvent/monomer mixture via exposure to a bright short UV pulse. Subsequently, the 3D sample can be scanned slowly by using confocal laser scanning microscopy (CLSM) with high accuracy, with the possibility of ?stitching? together very large 3D data volumes ($\sim$ 1500000 particles). This opens up the possibility to study nucleation and growth at high and low supersaturation. We control the degree of supersaturation by using dielectrophoretic compression in an electric bottle cell, where the arrest can be done at different moments of nucleation in the same sample. Here, we show the analysis of large nucleation data sets and discuss crystal symmetries, HCP/FCC ratios (HCP = hexagonal close-packed, FCC = face-centered cubic), density distributions, total and local volume fractions and look at the connection of these properties to the shape and size distribution of the nucleus.

SA24 Stimuli-responsive hierarchical self-assemblies of DNA-polymer hybrids

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Chemical functionality and shape anisotropy in colloidal particles hold a great promise to provide new programmed approaches of self-assembly. Here, inspired by the hierarchical self-assembly concept with block copolymers and exploiting the unique DNA's physicochemical properties, a novel family of DNA-polymer hybrids is constructed. These stimuli-responsive hybrids consist of a charged rigid DNA and a neutral temperature-responsive flexible polymeric segment which are covalently connected. The polymeric patches and rod-like DNA backbone display charge and flexibility difference. Moreover, a chemical mismatch between DNA and the polymeric block results in tunable amphiphilicity. Thus, it is possible to reversibly switch between a disordered ensemble and different multidimensional nanostructures of increasing complexity simply by changing the temperature. The formation of different self-assembled structures can be identified by small angle X-ray scattering (SAXS). SAXS measurements have been carried out in aqueous solutions of DNA-polymer hybrids and revealed phases ranging from lamella to cubic morphologies. Additionally, Brownian dynamics simulations provide a deeper insight into the molecular organization of cubic network phases. The results of this work show that the self-assembly approach presented here can be applied to different DNA architectures and significantly contribute to the structural DNA nanotechnology field.

SA25 Self-assembly of chiral mesophases from block copolymers using particle-based simulations

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Ordered network materials, such as the double gyroid, are comprised of two interwoven networks embedded in a matrix and can be formed via the self-assembly of block copolymers. Using a triblock copolymer, one can form an alternating gyroid thereby breaking network symmetry and resulting in a structurally chiral morphology. In this talk, we investigate the self-assembly of model achiral block copolymers into gyroid morphologies using coarse-grained molecular simulation. By co-assembling with a selective homopolymer, the thermodynamic stability of the morphology is further improved. The geometric topology is quantified, and the effect of varying volume fraction on net chirality is explored.

SA26 Stimuli Responsive Nematic and Smectic Liquid-crystalline Orders in Suspensions of Colloidal Ellipsoids Studied by SAXS

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We report a Small-Angle X-ray Scattering (SAXS) study of field-induced colloidal self-assembly of core-shell magnetic ellipsoids. Being made up of hematite cores and silica shells, these particles align in a direction perpendicular to the external magnetic field. For particles with smaller aspect ratio, $\rho = 2.8$, we observe four different self-assembled phases - oriented glass, smectic, nematic and para-nematic, as a function of the sedimentation-induced variation of the local particle concentration. Out of these four phases, smectic phase has never been predicted before for ellipsoidal particles. Further, in the smectic phase, an interesting peak shape was observed with highly anisotropic tails in the longitudinal direction (along the smectic periodicity) that can be rationalized by the variation of the structure factor in the form of a cylinder. The application of an external field freezes one of the rotational degrees of freedom; promoting non-centrosymmetric interparticle interactions and thereby confining the particles in 2D, which is turn leads to the variation of the structure factor in cylindrical shape in Fourier space. For particles with larger aspect ratio, $\rho = 3.7$, we observe a para-nematic phase along with a nematic one. In spite of the prolate shape of the particles, all the aforementioned phases are of oblate type. The mere fact that the external field align the short axes of the particles is responsible for this very interesting feature.

SA27 Self-assembled gels of Fmoc and P3HT

Santanu Kundu (Mississippi State University); Wijayapala,Rangana (Mississippi State University); Lakdusinghe,Madhubhashini (Mississippi State University); Hashemnejad, Meysam(Mississippi State University)

Molecular gels are of significant interest because of their potential applications in drug delivery, tissue engineering, sensors, etc. Here, we consider molecular gels formed by self-assembly of di-Fmoc-l-lysine (di-Fmoc) and P3HT in various organic solvents and water-organic solvent mixtures. Di-Fmoc forms stable gels in the water-organic solvent mixtures and the microscopy results capture fibrous structure in these gels. These long fibers topologically interact to form a gel-like material. The elastic modulus (G?) has been found to be a function of gelator volume fraction (ϕ). We obtained $G' \sim \phi^{1.8}$, having similarities with entangled polymer networks. We have also captured the di-Fmoc mediated gelation of P3HT in chloroform. The UV-vis spectroscopy and microscopy study elucidate the structural change and self-assembly process in this gel. The rheological behavior of these gel samples has been investigated by using cavitation rheology experiments. This technique is suitable for the gel samples in volatile solvents, as conducting traditional shear-rheology experiments on these samples can lead to drying of samples. The conductivity of these gels has been investigated both in dry and wet conditions.

SA28 Effects of confinement on self-assembly in systems with competing interactions

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Systems with competing interactions, such as mixtures of surfactants, lipids, diblock copolymers and colloids, are widespread in nature and have relevance in biology and industry. Despite the different chemical identity of their components, all these systems behave in a similar way in bulk and exhibit phase diagrams with the same topology. Phases such as lamellar, hexagonal, and cubic triply periodic have been observed in all those systems. We study the behavior under confinement of nanoparticles interacting via the short-range attraction and long-range repulsion potential (SALR) by means of Grand Canonical Monte Carlo simulations. We found that the confinement may significantly change the morphology of the bulk phases. In particular, we have observed the formation of many different helical structures in cylindrical pores for different pores sizes. The results of our work might be of interest to engineers and scientists. It can be exploited to the development of new materials and it may help to understand the formation of similar structures in living organisms.

SA29 On the Role of Flexibility in Linker-Mediated DNA Hydrogels

STOEV, Iliya (University of Cambridge)

”Three-dimensional DNA networks, composed of trivalent or tetravalent nanostars with sticky, single-stranded DNA overhangs, have been previously studied in the context of designing thermally responsive, viscoelastic hydrogels. In this work we use linker-mediated gels, where the sticky ends of two trivalent nanostars are connected through the complementary sticky ends of a linear DNA duplex. We can design this connection to be either rigid or flexible by introducing flexible, non-binding bases. The additional flexiblity provided by these non-binding bases influences the effective elasticity of the percolating gel formed at low temperatures. (1) Here we show that by choosing the right length of the linear duplex and non-binding flexible joints, we obtain a completely different phase behaviour to that observed for rigid linkers. In particular, we use dynamic light scattering as microrheological tool to monitor the self-assembly of DNA nanostars with linear linkers as a function of temperature. (2) While we observe classical gelation when using rigid linkers, the presence of flexible joints leads to a cluster fluid with reduced viscosity. Using oxDNA to investigate the nanostar-linker topology, we hypothesise on the possible structure formed by the DNA clusters.

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SA30 Irreversible aggregation with two time scales

TAVARES, Jos M. (Centro de Fsica Teórica e Computacional Faculdade de Cincias, Universidade de Lisboa and Instituto Superior de Engenharia de Lisboa);

The classical Smoluchowski equation has analytical solutions for constant, additive and multiplicative kernels but, in all these cases, a single rate constant (or time scale) for aggregation is assumed. Inspired by processes in bioengineered systems - where the components have very different diffusion constants - we study the irreversible aggregation of f-functional (slow) particles mediated by bifunctional (fast) monomers or linkers. We generalize Smoluchowski equation to include two time scales and solve it for two types of kernels. We obtain -as a function of f, of the ratio ϕ between the concentrations of linkers and particles, and of the ratio α between the two time scales- analytical expressions for the cluster size distribution, for the percolation threshold and for some scaling relations between different bond probabilities. Numerical calculations reveal that the percolation time varies strongly with both α and ϕ, and that for each ϕ there is an α that minimizes it.

SA31 Templating the twist-bend nematic liquid crystal phase

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Liquid crystals are a fascinating class of materials that elegantly combine characteristics of the conventional solid and isotropic liquid states. Over recent years, templating of various liquid crystal phases using polymers has sparked research interests as it offers great potential in understanding interfacial interactions between liquid crystals and polymers at the nanoscale.

This work focuses on templating of one of the most fascinating liquid crystal phases ? the twist-bend nematic phase. In the twist-bend nematic phase, the liquid crystals assemble into a heliconical structure with a nanometre pitch [1,2] by the spontaneous twisting and bending of the director in space, which is extraordinary as the constituent liquid crystals are achiral in nature. Twist-bend nematic liquid crystals provide promising applications in fast-switching photonic and electro-optic devices. However, understanding the mechanical and electrical properties of this phase is difficult in conventional twist-bend nematic materials due to its high viscosity. [3?5] In this presentation, a detailed study of the elastic, dielectric and electro-optic behaviour of templated twist-bend nematic phases refilled with a nematic mesogen will be discussed.

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SA32 Structure and thermodynamics of elliptic patchy particles

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"In an effort to investigate colloidal particles that feature both shape anisotropy as well as surface decorations we put forward a novel model for elliptic patchy colloids. Considering a two-dimensional geometry, the bodies of our particles are impenetrable ellipses (of aspect ratio κ) that can be decorated on their (co-)vertices by up to four patches. The latter ones range over a certain patch amplitude θ on the surface of the osculating circles defined for the (co-)vertices of the ellipse. The opening angle of the patches is limited by the accuracy with which the osculating circle represents the elliptic surface. Within the patch region the interaction is assumed to be constant in depth and range. Thus our model can be considered as a straightforward extension of the Kern-Frenkel model for circular (spherical) patchy particles [1].

In order to use this model in Monte Carlo simulations we have used (i) for the undecorated bodies of our particles the overlap criterion of two ellipses put forward by Vieillard-Baron [2] and (ii) the patch-patch interaction criterion used for the original Kern-Frenkel model. Using 1~260 particles in Monte Carlo simulations in the isobaric-isothermal and in the canonical ensemble, we have studied the spatial and the orientational order as well as the equation-of-state. In an effort to better accommodate the emerging ordered phases we have used a simulation box which can vary both in shape and in area. Following previous investigations on undecorated elliptic particles [3] we have considered three κ values, namely $\kappa = 2, 4$ and 6.

Varying systematically the pressure and the temperature and choosing different patch decorations we investigate the emergence of the disordered and the ordered phases, which are the result of a trade-off between energetic and entropic contributions to the thermodynamic potential. The ordered particle arrangements were classified using the spatial radial distribution and suitably chosen orientational correlation functions [3] and appropriate order parameters: in particular we were interested in the occurrence of the nematic phases, of plastic crystals and of hexatic phases.

First results for the structure and the equation of state for a system of particles with two symmetric patches located at the co-vertices have been published recently [4].

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SA33 Self Assembly

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Colloidal nanorods made of semiconductors or noble metals exhibit useful and tuneable properties that depend on their dimensions and on how they are ordered on larger scales. [1] How they assemble is highly dependent on how the rods interact with one another and with their environment. One way to drive the assembly of nanorods into an ordered structure is via the addition of a polymer depletant. [2] Adding this depletant applies an osmotic pressure to the rods causing them to aggregate into liquid-like droplets or ordered assemblies (nematic, smectic or crystal), depending on the dimensions and the concentrations of the two components.

To better understand the forces driving assembly in such systems, we have used SAXS experiments together with Monte-Carlo simulations to study rod assembly in dispersions of CdSe nanorods and polystyrene depletants of different molecular weights. We find that, depending on the polymer size, some types of order do not form, different types of order may coexist over large concentration ranges and the dimensions of an assembly can change the order present. Our results indicate that this is due to interfacial contributions to the free energy, which strongly affect the order and shape of the assemblies that form.

Finally, we have used umbrella sampling to characterise assembly pathways for a range of different polymer concentrations and sizes, and show that monolayer nucleation and growth can be the optimal pathway even when starting from a dense liquid state.

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SA34 A grating-aligned shock-resistant ferroelectric liquid crystal electro-optic shutter with sub-millisecond response times

WYATT, Peter James McCormack (University of Leeds (SOFI CDT)); BAILEY, James (Dynamic Vision Systems LTD); NAGARAJ, Mamatha (University of Leeds); JONES, J. Cliff (University of Leeds)

Ferroelectric liquid crystals (FLCs) were a highly promising research subject for the display industry in the 1980s and 1990s, due to their sub-millisecond switching times and inherent bistability. The Surface Stabilised FLC [1] seemed suited as an alternative to nematic-based liquid crystal displays (LCDs) since high complexity passive displays could be made without thin-film-transistors at each pixel [2]. Uniform alignment of the tilted smectic layers of the FLC must be retained even after mechanical shock to the display. However smectic liquid crystals are susceptible to shock induced flow, rendering them unsuited for large area displays. These fast switching speeds still remain desirable, for instance allowing frame sequential colour in projector display applications. Liquid Crystal on Silicon (LCoS) spatial light modulators based on FLCs are commercially successful and are less sensitive to shock, but new shock-insensitive modes are still important to develop.

A simple but novel geometry for FLC electro-optic shutters is presented, based on low-amplitude, low-pitch surface-relief gratings and interdigitated electrodes (IDEs) to controllably align the FLC c-director (the unit vector describing the direction of the molecular tilt within the smectic layer). The gratings are surface treated to induce a homeotropic, or vertical, alignment to the FLC layer normal, k, which is parallel to the substrate normal. Such alignments are shown to exhibit greater shock stability due to the initial alignment of the smectic layers relative to the direction of the induced liquid flow. The surface-relief grating provides a preferred orientation for the c-director to which it returns after a mechanical shock or electrical addressing, seemingly self-healing. When addressed with IDEs, sub-millisecond response times are obtained. This relatively simple geometry has led to a working prototype that demonstrates both resistance to mechanical shock as well as sub-microsecond switching times. Improvements are suggested that will help optimise the device for use in LCoS spatial light modulators, high-speed adaptive optics and head-mounted displays for virtual/augmented reality.

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SA35 Phantasmagoric liquid crystals

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We have found the new types of the continuous isotropic(I)-nematic(N) transition originated from the shape transformation of micelles in extremely dilute lyotropic nematic (LN)($\phi \sim 3$ 9wt%). For thermotropic nematic (TN), orientation order is only broken by the order-disorder transition above weak but first order I-N transition keeping the anisotropy of the ?building blocks? which is equivalent to the rod like one molecule. On the contrary, even the shape of building blocks can be deformed dependent on temperature, concentration or other thermodynamic quantities in LN. The birefringence continuously weakens towards the I-N transition due to the decrease in order parameter as well as in the simultaneous decrease in anisotropy of the building blocks. We have investigated the I-N phase transition phenomena by polarizing microscope, dynamic light scattering, flow birefringence and viscosity measurement. LN phase is formed by a combination of anionic and cationic surfactants (sodium dodecyl sulfate; SDS and dodecyl trimethyl ammonium bromide; C12TAB, respectively) at a total surfactant concentration between $3wt\% \leq \phi \leq 9wt\%$. The weight fraction α between SDS and C12TAB is varied between 2.0 and 2.7. With decreasing α, the surface change of micelle is compensated, and the micelles is easy to deform the rod or sheet structure rather than spherical micelle. We measured the temperature dependece of the relaxation frrequency by VH and VV modes in DLS measurement. Relaxation time of orientation fluctuation observed by VH mode diverges just on TIN (23C), which is identification of the continuous I-N transition. On the contrary, it is evident that the characteritic time of diffusion of micelles observed by VV mode (green circles) shows the slow down phenomena around another phase transition temperature (21C) slightly lower than TIN. Finally, we constructed precise phase diagram. Nematic phaes can be stablized in extremely dilute regime ($\phi < 3\%$).

SA36 Self-assembly in magnetic filament systems of different topologies: influence of additional central interaction

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Magnetic filament systems (semiflexible polymer-like chains of magnetic nanoparticles permanently crosslinked with polymers) have been recently pointed as promising building blocks for the creation of magnetoresponsive materials. The synthesis and control of the properties of these systems has experienced a great progress in recent years thanks to the enhancement of polymer crosslinking techniques. The fundamental understanding of the self-assembly properties of colloidal systems is one of the key topics in current research on novel microstructured soft materials and technologies. In this work we investigate self-assembly of magnetic filaments of different topology with additional central interaction. We performed molecular dynamic simulations using a Langevin thermostat. Cluster analysis based on graph theory is used to analyze the obtained data. We discovered, that additional attraction quantitatively changes the self-assembly scenario. The difference in topologies does not affect on self-assembly of magnetic polymer dispersions. Magnetic interaction influences on an internal structure of organized clusters, but does not change the self-assembly scenario. All these results will pave the way for the development of analytical models and identify the most interesting building block candidates for the design of new magnetoresponsive materials.