



Conference

Physics of Complex Colloids

Book of Abstracts

Ljubljana May 14-18 2013

organized by Jožef Stefan Institute and University of Ljubljana

edited by N. Osterman and P. Ziherl

cover design A. Šiber

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Preface

It is our pleasure to welcome you to the *Physics of Complex Colloids* conference. Organized within the Marie Curie Initial Training Network COMPLOIDS, the conference is the main scientific meeting of the network. During the past decade, colloidal science has witnessed a rapid development epitomized by, e.g. active colloids or the ever more elaborate control of colloids by external fields. Increasingly more closely linked to other branches of soft-condensed-matter physics as well as with biophysics, colloids are discussed at many meetings of more general nature, and this has proved very productive. On the other hand, a focused forum dedicated to the recent advances in the experimental, theoretical, and applied studies of colloids may well promote the exchange within the field more efficiently, thereby contributing to its consolidation and the cross-pollination of ideas. The aim of the *Physics of Complex Colloids* conference is to provide such an opportunity by reviewing the most exciting new results, the novel techniques, and the concepts.

With sessions on rheology, colloids in external fields, self-assembly, arrested states, liquid-crystal colloid dispersions, active colloids, and applications, the conference accurately reflects the current stage of soft matter science and colloidal physics. The tone of the sessions will be set by 14 invited lectures, and 28 contributed lectures will highlight the most captivating recent results. The poster session with 83 posters will hopefully foster a broad discussion and help to understand the details of studies presented. With the open style of the *Physics of Complex Colloids* conference, we aim at creating an atmosphere where both students and established researchers will feel equally welcome. Let us know whether we succeeded.

This conference would not be possible without the funding of the European Commission through the Marie Curie Actions program. We are also grateful for the support of the Jožef Stefan Institute, the University of Ljubljana, and the Slovenian Research Agency.

Thank you for participating at the conference and for contributing to its scientific contents. We hope that you will like it, and we wish you a productive and enjoyable stay in Ljubljana.

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University of Ljubljana
Local Organizing Committee

Christos N. Likos
Universität Wien
International Scientific Committee

Committees

International Scientific Committee

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Primož Ziherl (University of Ljubljana, Slovenia)
Slobodan Žumer (University of Ljubljana, Slovenia)

Practical Information

Venue

The conference will take place in the Cankarjev dom Cultural and Congress Centre (Prešernova 10, SI-1000 Ljubljana, Slovenia). All lectures will be held in the Kosovel Hall in Foyer II.

Registration

The registration desk is located in Foyer II of the Cankarjev dom Cultural and Congress Centre. Registration starts on Tuesday May 14 2013 at 14.00.

On Wednesday May 15 2013 the conference office will open at 8.00. From Thursday May 16 2013 until Saturday May 18 2013 the office will open at 8.30. Every day the office will be closed 15 minutes after the last scientific event.

Upon registration, you will receive

- Book of Abstracts,
- name badge, and
- certificate of attendance.

We ask you kindly to wear the name badge at all scientific and social events of the conference. Only participants wearing the badge will be admitted to the lecture hall, coffee breaks, welcome reception, and conference dinner.

The registration fee includes

- admittance to all lectures and the poster session,
- conference material, and
- welcome reception, conference dinner, and coffee breaks.

Lunch is not included in the registration fee. A map with a list of nearby restaurants is enclosed in the registration bag.

Internet

Free on-site wireless access to internet is provided throughout the duration of the conference. The name of the network is CDWLAN. No login or password is needed.

Contact

Local Organizing Committee: P. Ziherl, Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia; phone: +386 1 4773 613 or +386 41 315 341, email: comploids2013@fmf.uni-lj.si.

Congress Agency: A. Kregar, Cankarjev dom Cultural and Congress Centre, Prešernova 10, SI-1000 Ljubljana, Slovenia; phone: +386 1 2417 133, fax: +386 1 2417 296, email: alenka.kregar@cd-cc.si.

Presentations

Oral Presentations

Speakers can use their own laptops but are urged to test their presentation at least a day in advance during one of the breaks so as to ensure that the presentation is fully functional. During the break before their session, the speakers are asked to connect to the projector.

A backup Windows laptop will be available to speakers.

The duration of both invited and contributed lectures is 30 minutes including a 25 minute presentation and a 5 minute discussion.

Poster Presentations

The poster session will take place in Foyer II on Thursday May 16 2013 from 16.00 until 18.00. The posters will be arranged alphabetically by the last name of the presenting author, and each poster should be displayed on the board labeled by the poster code indicated in the book of abstracts (e.g. P61). The posters should be displayed no later than during the lunch break on Thursday May 16 2013. The authors are encouraged to display the posters throughout the duration of the conference. The posters should be removed at the end of the conference.

During the poster session, the presenting authors are kindly asked to stay close to their poster.

Social Program

Welcome Reception

The welcome reception will take place on Tuesday May 14 2013 from 19.00 until 21.00 in Foyer II of the Cankarjev dom Cultural and Congress Centre. Snacks and drinks will be served.

Conference Dinner

The conference dinner will be held on Friday May 17 2013 at 20.00 in CD Club located on the 5th floor of the Cankarjev dom Cultural and Congress Centre.

Program

Wednesday May 15 2013

8.50 Opening

9.00-10.30 Active Colloids I (chair: C. Bechinger)

- 9.00 *Z. Dogić: Hierarchical active matter: From extensible bundles to active gels, streaming liquid crystals and motile emulsions*
- 9.30 I. Buttinoni: Clustering transition and phase separation of a self-propelled colloidal suspension
- 10.00 W. C. K. Poon: The physics of a growing bacterial colony

10.30-11.00 Coffee Break

11.00-12.30 Self-Assembly I (chair: M. A. Miller)

- 11.00 *R. van Roij: Charge-regulating and patchy colloids in aqueous and oily electrolytes*
- 11.30 L. Di Michele: Multistep kinetic self-assembly of DNA-coated colloids
- 12.00 R. Matthews: Influence of fluctuating membranes on self-assembly of patchy colloids

12.30-14.30 Lunch Break

14.30-16.00 Rheology I (chair: M. M. Telo da Gama)

- 14.30 *R. Yamamoto: Simulations of colloids and self-propelled particles with fully resolved hydrodynamics*
- 15.00 N. Bruot: Synchronization of colloidal rotors modeling cilia or flagella
- 15.30 M. Ravnik: Controlling active and passive nematic flow in microfluidic channels

16.00-16.30 Coffee Break

16.30-18.00 Arrested States I (chair: T. Schilling)

- 16.30 *L. Cipelletti: Dynamics of colloidal gels and glasses under gravitational stress*
- 17.00 Y. Chushkin: Anisotropic dynamical heterogeneity
- 17.30 C. Valeriani: Avalanches during crystallization of a glass of hard spheres

Thursday May 16 2013

9.00-10.30 Colloids in External Fields (chair: W. C. K. Poon)

- 9.00 *B. Rotenberg: Charging of nanoporous carbon electrodes: The molecular origin of supercapacitance*
- 9.30 P. Keim: Phase transition in a 2D colloidal system far from equilibrium
- 10.00 A. Reinmüller: Static and dynamic colloidal organization induced by electrolyte gradients

10.30-11.00 Coffee Break

11.00-12.30 Liquid-Crystal Colloid Dispersions I

(chair: N. M. Silvestre)

- 11.00 *I. Mušević: Nematic colloids: Topology and photonics*
- 11.30 P. van der Schoot: Connectedness percolation in complex colloid mixtures
- 12.00 P. Cluzeau: Self organization process in meniscus of smectic-C free-standing films

12.30-14.30 Lunch Break

14.30-16.00 Active Colloids II (chair: U. Jonas)

- 14.30 *H. Stark: Active motion under external fields and in confinement*
- 15.00 A. Brown: Back to front and upside down: Reversible motion and gravitaxis in simple catalytic swimmers
- 15.30 P. B. S. Kumar: Autonomous motility and beating in semi-flexible active filaments

16.00-18.00 Poster Session

Friday May 17 2013

9.00-10.30 Self-Assembly II (chair: G. Kahl)

- 9.00 *I. Kretzschmar: Electric and magnetic-field assembly of Janus and patchy particles*
- 9.30 B. Capone: Telechelic star polymers as self-assembling units from the molecular to the macroscopic scale
- 10.00 M. Schmiedeberg: Stability, growth, and dynamics of colloidal quasicrystals

10.30-11.00 Coffee Break

11.00-12.30 Arrested States II (chair: P. S. Clegg)

- 11.00 *B. Ruzicka: Multiple arrested states in a charged colloidal system*
- 11.30 P. Mohanty: Soft colloids with tunable interactions – microgels as models for soft dipolar fluids
- 12.00 P. Kwasniewski: Probing dynamics of hard sphere suspensions at high volume fractions with coherent X-rays

12.30-14.30 Lunch Break

14.30-16.00 Active Colloids III (chair: D. Frenkel)

- 14.30 *A. Snezhko: Emergent dynamics and self-assembly in field driven active colloids*
- 15.00 C. Maggi: The unexpected behaviour of swimming-cells systems under the influence of external force fields
- 15.30 I. Pagonabarraga: Emergent structures of active colloid suspensions under gravity

16.00-16.30 Coffee Break

16.30-18.00 Applications (chair: F. G. Lo Verso)

- 16.30 *K. Velikov: Application of complex colloids in fast moving consumer goods*
- 17.00 *H. Bodiguel: Microfluidics: A nice tool to study oil enhanced recovery processes*
- 17.30 J. Yamamoto: Liquid-crystalline nanomicelles for active drug delivery system

20.00-23.00 Conference Dinner

Saturday May 18 2013

9.00-10.30 Rheology II (chair: S. Kantorovich)

- 9.00 *S. Fielding: Ageing and flow instability in soft glassy materials*
- 9.30 N. Lin: Nonlinear coupling in biaxially sheared dense colloidal suspensions
- 10.00 G. Foffano: Simulations of colloids in active fluids: Negative drag and aggregation properties

10.30-11.00 Coffee Break

11.00-12.30 Liquid-Crystal Colloid Dispersions II

(chair: P. Cluzeau)

- 11.00 A. Giacometti: The isotropic-to-nematic phase transition in hard helices: Onsager-like theory and Monte Carlo simulation
- 11.30 N. Hijnen: Using partially miscible solvents to control colloidal stability and the assembly of colloidal rods
- 12.00 D. Beller: Modeling the assembly of colloids with sharp features in nematic liquid crystals

12.30-14.30 Lunch Break

14.30-16.00 Self-Assembly III (chair: A. Šiber)

- 14.30 *E. Bianchi: Inverse patchy colloids: Effect of the interplay between attractive and repulsive anisotropic interactions on the collective behaviours*
- 15.00 T. Vissers: Computer simulations of attractive one-patch colloids
- 15.30 P. Varilly Alvarado: Valency without patches: Many-body effects in DNA-coated colloids

16.00 Closing

Lectures

Active Colloids I

chair C. Bechinger

Hierarchical active matter: From extensible bundles to active gels, streaming liquid crystals and motile emulsions

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Laws of equilibrium statistical mechanics impose severe constraints on properties of conventional materials. For example, equilibrium materials assembled from inanimate components cannot perform work and thus never exhibit autonomous motility. To overcome these restrictions, recent attention has focused on studying far-from-equilibrium materials assembled from animate microscopic objects. The emerging field of active matter promises an entirely new category of materials, with highly sought after properties such as autonomous motility and internally generated flows. In this vein, I describe recent experiments that have focused on reconstituting dynamical structures from purified biochemical components. In particular I will describe recent advances that include: (i) study of 2D active nematic liquid crystals whose streaming flows are determined by internal fractures and self-healing as well as spontaneous unbinding and recombination of oppositely charged disclination defects, (ii) reconstitution of active gels characterized by highly tunable and controllable spontaneous internal flows, and (iii) assembly of active emulsions in which aqueous droplets spontaneously crawl when in contact with a hard wall. The key unifying property that permeates all these materials are spontaneous flows and/or motion, which occurs in the absence of any external field.

Clustering transition and phase separation of a self-propelled colloidal suspension

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Living active systems such as bacterial solutions or flocks of birds show interesting collective phenomena which are only poorly understood. In order to obtain some fundamental understanding, we try to mimic similar processes in systems of artificial swimmers which have been already shown to exhibit striking similarities with biological systems. By means of a recently developed phoretic swimmer-system whose propulsion can be controlled by the incident light intensity, we study the complex dynamics of clustering which occurs in dense suspensions of swimmers. At low densities we observe the formation of small dynamic clusters, whose size and shape continuously varies due to collisions and rotational diffusion. At higher densities and large propulsion speeds the active suspension undergoes a disorder-order phase transition and separates into few big clusters and a diluted gas phase. Numerical simulations suggest that both the clustering and the phase separation can be explained by the self-trapping of particles undergoing head-on collisions.

The physics of a growing bacterial colony

W. C. K. Poon, D. Dell'Arciprete, F. Farrell, B. Waclaw, D. Marenduzzo

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We study experimentally the structure and dynamics of a colony of growing *E. coli* bacteria confined to 2D. Each bacterium, a 2:1 spherocylinder, doubles and then divides. We measure the decay of angular correlation between cells within the colony, track the origin and dynamics of topological defects, and measure the growth rate of individual cells. Based on comparison with simulations, we draw analogies with the equilibrium phase behaviour of hard rods, and propose a new coarse-grained model treating growth as an internal alignment field.

Self-Assembly I

chair M. A. Miller

Charge-regulating and patchy colloids in aqueous and oily electrolytes

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The class of anisotropic colloidal (nano)particles and patterned surfaces is extremely versatile nowadays due to enormous advances in the colloidal synthesis. These particles break the rotational symmetry of classical spherical particles by e.g. protrusions or an inhomogeneous (patchy) distribution of chargeable groups on the surface. Examples include Janus particles with two chemically different hemispheres, or planar surfaces with chemical stripe or checkerboard patterns. The electrostatic interaction between pairs of these objects is often totally different from what DLVO theory (for homogeneous surfaces) would predict. In the first part of this talk we will extend the traditional monopole-monopole interaction of DLVO theory towards monopole-dipole, dipole-dipole, etc., taking into account the nonlinear coupling of the electrostatic multipoles and extending the concept of Alexander's charge renormalization to multipoles [1, 2]. The electrostatic interaction between colloidal particles is not always described properly by a fixed surface charge; one often needs to account for charge regulation due to the response of the surface chemistry to changes in the environment [3]. This has important consequences for patched particles. In the second part of this talk we will couple charge regulation mechanisms to patchy surfaces, calculating the resulting heterogeneous surface charge and the deformed ionic double layers. We will see that (i) small patches often acquire a relatively high charge density and (ii) charge regulation can induce a dominant short-range attraction between patched surfaces that repel each other at large distances [3]. In the third part of the talk, we will focus on an extreme case of charge

regulation, as described by constant-zeta-potential conditions [4]. We will show that this mimics the double role of (micellar) ions in extremely apolar (oily) solvents, where they not only act as screening agents but also as surface chargers due to adsorption onto the colloidal surfaces. We will show that this can give rise to fluid-crystal-fluid-crystal phase sequences of colloidal suspensions upon increasing the ionic strength. Combining this with a new and simple freezing criterion for charged spheres yields quantitative agreement with recent experiments [5].

- [1] N. Boon, E. Carvajal Gallardo, S. Zheng, E. Eggen, M. Dijkstra, and R. van Roij, *J. Phys.: Condens. Matter* **22**, 104104 (2010).
- [2] J. de Graaf, N. Boon, M. Dijkstra, and R. van Roij, *J. Chem. Phys.* **137**, 104910 (2012).
- [3] N. Boon and R. van Roij, *J. Chem. Phys.* **134**, 054706 (2011).
- [4] F. Smallenburg, N. Boon, M. Kater, M. Dijkstra, and R. van Roij, *J. Chem. Phys.* **134**, 074505 (2011).
- [5] N. Boon, M. Dijkstra, F. Smallenburg, and R. van Roij, in preparation.

Multistep kinetic self-assembly of DNA-coated colloids

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Self-assembly is commonly described as the process through which a system, initially in a disordered configuration, evolves towards an equilibrium ordered phase driven only by local interactions. This definition is too restrictive. Nature provides examples of amorphous, yet functional, materials assembled by kinetically arresting the equilibration process [1, 2]. An example is given by the keratin/chitin sponge-like structures providing structural coloration to the feathers of some species of birds [1] or beetles [2]. Equilibrium self-assembly relies uniquely on the local interactions to determine the target structure. The key drawback of this approach lies in the difficulty of designing interactions strong enough to induce ordering, yet weak enough to make equilibration feasible. Kinetic self-assembly does not suffer from this issue. Controlling both the interactions and the pathway to kinetic arrest to select the target structure, in fact, it is intrinsically more reliable and flexible than its equilibrium counterpart. We propose a novel strategy to direct the gelation of two-component colloidal mixtures by sequentially activating selective inter-species and intra-species interactions [3]. We investigate morphological changes in the structure of the arrested phases by means of molecular dynamics simulations and experimentally using DNA-coated colloids (DNACCs). The selectivity and the sharp thermal activation of hybridization-

mediated interactions make DNACCs ideal for the purpose of this work [3, 4]. To demonstrate the potential and flexibility of our scheme, we describe two model systems. The first binary mixture undergoes a two-step gelation, with the second aggregating phase forced to gel in the confined environment produced by the first aggregating phase. The second system self-assembles into core-shell colloidal gels, with the second component coating the first-formed network, which acts as a scaffold. In both cases, by modifying the quenching procedure leading to two-step kinetic arrest and the concentration ratio of the two components, a rich range of morphologies can be obtained [3]. Colloidal structures assembled via DNA can be made permanent, allowing application of our strategy to the self-assembly of functional materials. It will be possible to replicate natural amorphous photonic structures for structural coloration [1, 2], with applications in paints, coatings and display technology. The use of materials with different refractive indices for different components will allow fine tuning the optical response. In hybrid photovoltaics, controlled phase separation is required between polymer acting as donor and inorganic particles acting as acceptors [5]. Our core-shell self-assembly can be adapted to build inorganic scaffolds of different morphology and coat them with organic particles.

- [1] B. Q. Dong, T. R. Zhan, X. H. Liu, L. P. Jiang, F. Liu, X. H. Hu, and J. Zi, *Phys. Rev. E* **84**, 011915 (2011).
- [2] H. Yin, B. Dong, X. Liu, T. Zhan, L. Shi, J. Zi, and E. Yablonovitch, *Proc. Natl. Acad. Sci. USA* **109**, 10798 (2012).
- [3] L. Di Michele, F. Varrato, S. H. Nathan, J. Kotar, G. Foffi, and E. Eiser, in preparation.
- [4] F. Varrato, L. Di Michele, M. Belushkin, N. Dorsaz, S. H. Nathan, E. Eiser, and G. Foffi, *Proc. Natl. Acad. Sci. USA* **109**, 19155 (2012).
- [5] U. Bach, D. Lupo, P. Comte, J. E. Moser, F. Weissortel, J. Salbeck, H. Spreitzer, and M. Grätzel, *Nature* **395**, 583 (1998).

Influence of fluctuating membranes on self-assembly of patchy colloids

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A coarse-grained computational model is used to investigate the effect of a fluid membrane on patchy-particle assembly into biologically-relevant structures motivated by viral cores and clathrin. For cores, we demonstrate a non-monotonic dependence of the promotion of assembly on membrane stiffness. If the membrane is significantly deformable, cores are enveloped in buds, although this effect is suppressed for very flexible membranes. In the less deformable regime, we observe no marked enhancement for cores, even for strong adhesion to the surface. For clathrin-like particles, we again observe the formation of buds, whose morphology depends on membrane-flexibility.

Rheology I

chair M. M. Telo da Gama

Simulations of colloids and self-propelled particles with fully resolved hydrodynamics

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Using the smoothed profile method (SPM) method [1, 2] developed for direct numerical simulations (DNS) of colloidal dispersions, we studied several dynamical problems of particle dispersions, including their rheological behaviours under steady and oscillatory shear flows. Recently, SPM is extended for dispersions of self-propelled particles by replacing the non-slip boundary condition (usual for colloids) with an actively slip boundary condition (to model squirmers) at the fluid/particle interface. Several dynamical behaviours of the hydrodynamically interacting self-propelled particles will be discussed [3, 4].

- [1] Y. Nakayama, K. Kim, and R. Yamamoto, Eur. Phys. J. E **26**, 361 (2008).
- [2] KAPSEL website, <http://www-tph.cheme.kyoto-u.ac.jp/kapsel/>
- [3] R. Tatsumi and R. Yamamoto, Phys. Rev. E **85**, 066704 (2012).
- [4] J. Molina, Y. Nakayama, and R. Yamamoto, preprint.

Synchronization of colloidal rotors modeling cilia or flagella

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We use colloidal particles driven by optical tweezers to understand the emergence of synchronization of oscillators present in the living world, such as cilia or flagella. In our experimental model, a single cilium is represented by a spherical colloidal silica bead. The particles are driven along circular trajectories, either by keeping the position of a trap ahead of the particle's position (Cambridge), or by using holographic tweezers (Bristol). We show experimentally that two oscillators synchronize in phase. Two models have been proposed to explain the synchronization through hydrodynamic interaction: The Lenz and Golestanian models. In the Lenz model [1], synchronization arises from the possible deviation of the position from the expected circular trajectory. The ability to deviate from the trajectory is described by an elastic restoring force acting in the direction orthogonal to the trajectory. On the other hand, the Golestanian model [2] explains the relation between the profile of the driving force along the circular path and the strength of synchronization. We discuss, with experiments supported by numerical simulations, the contribution of each effect to the strength of synchronization depending on the parameters of the oscillators, in particular the elastic stiffness and the force profile.

[1] T. Niedermayer, B. Eckhardt, and P. Lenz, *Chaos* **18**, 037128 (2008).

[2] N. Uchida and R. Golestanian, *Phys. Rev. Lett.* **106**, 058104 (2011).

Controlling active and passive nematic flow in microfluidic channels

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The flow in confined geometries is relevant in fields ranging from microfluidic lab-on-the-chip devices to active systems of biological matter. In complex fluids with internal orientational order, the material flow is coupled to the deformations of the orientational order via internal material stress. Technologically, this coupling offers an interesting driving mechanism for controlling the material flow, whereas in biological materials, this coupling is central in the ordering and active locomotion mechanism. Here, we present a numerical study of active and passive nematic flow in microfluidic channels. The active and passive liquid crystal materials are different in origin, yet the coupling between the material flow and orientational order is generically similar. Our work is based on the phenomenological Beris-Edwards model, which is solved via a hybrid lattice-Boltzmann method in full three spatial dimensions. For passive LCs [1], we show the emergence of three characteristic flow regimes depending on the driving pressure. We demonstrate shaping of the material flow fronts by tuning the nematic orientational profiles, capable of flow-steering and multi-stream flows. Alternatively, for active LCs in channels [2], we show and discuss active flow states, which are found to importantly depend on the confinement and anchoring conditions by the surfaces. In a cylindrical capillary, we find that active flow emerges not only along the capillary axis but also, as the secondary flow, within the plane

of the capillary, where radial vortices are formed. Interplay between the primary and secondary velocities leads to a spiraling active flow field with a well-defined pitch moving down the capillary. We show that topological defects, imposed by heterogeneous boundary conditions, act as sources of activity – effective local pumps – driving the flow. We also show that measuring the magnitude of the active flow as a function of the capillary radius could be used to determine the value for the activity coefficient.

- [1] A. Sengupta, U. Tkalec, M. Ravnik, J. M. Yeomans, C. Bahr, and S. Herminghaus, *Phys. Rev. Lett.* **110**, 048303 (2013).
- [2] M. Ravnik and J. M. Yeomans, *Phys. Rev. Lett.* **110**, 026001 (2013).

Arrested States I

chair T. Schilling

Dynamics of colloidal gels and glasses under gravitational stress

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We use novel space and time resolved light scattering methods to investigate the dynamics of colloidal suspensions under gravitational stress. In the first part of my talk, I will discuss the behavior of colloidal gels, where the volume fraction is moderate ($\phi \sim 0.05-0.2$) and attractive interactions are induced via the depletion mechanism. I will show that a single parameter, the time dependent compressive strain rate, rules both the macroscopic settling of the gel and its microscopic dynamics [1]. Additionally, gels prepared at various volume fractions and interaction strength exhibit a universal behavior in that their asymptotic concentration profile can be scaled onto a master curve [2]. In the second part of my talk, I will discuss nearly neutrally buoyant suspensions of colloidal spheres, to which small amounts of fast-settling probe spheres are added. The focus will be on the volume fraction dependence of the suspension viscosity and its relationship with the structural relaxation time.

- [1] G. Brambilla, S. Buzzaccaro, R. Piazza, L. Berthier, and L. Cipelletti, Phys. Rev. Lett. **106**, 118302 (2011).
- [2] S. Buzzaccaro, E. Secchi, G. Brambilla, R. Piazza, and L. Cipelletti, J. Phys.: Condens. Matter **24**, 284103 (2012).

Anisotropic dynamical heterogeneity

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Glassy solids and liquids are in disordered state but their dynamical behaviour is remarkably different. The molecules diffuse freely in liquids but their motions in glasses become increasingly limited. The rapid slow down of the dynamics in liquids upon cooling is called a glass transition phenomena. The idea that such slowing down is related to the growing cooperative length scale in the system dates back to Adam and Gibbs [1]. The structural relaxation in a deep supercooled state is possible through correlated motions of “blobs” of particles. Such cooperativity results in strong temporal fluctuations of the dynamics. Experimentally temporal heterogeneity is accessible by measuring χ_4 , the variance of the time-resolved correlation function [2]. Recently it was shown that glass transition is accompanied by growing dynamic length scale [3]. In this work we focus on the dynamical heterogeneity in a colloidal glass of magnetic nanoparticles with repulsive interparticle interactions. This dense charge-stabilized dispersion is a model system that replicates the behaviour of a real molecular glass-former. Under an applied magnetic field, the interparticle interactions remains repulsive however becomes anisotropic [4]. The investigation of the effect of the magnetic field on the dynamics shows that the field induces a moderate structural but a very strong dynamical anisotropy in the glassy system. It also causes a highly anisotropic cooperativity, almost two orders of magnitude larger in the field direction than in the perpendicular direction or in zero field. The origin of the observed anisotropic dynamics is discussed.

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Avalanches during crystallization of a glass of hard spheres

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In the present work, we underline the role of avalanches (a subset of particles breaking out of their cages and undergoing large and correlated displacements) in unraveling the microscopic mechanism of high concentration, diffusionless crystallization from a constrained aged glass of monodisperse hard-spheres. For these amorphous states, constrained ageing causes an enhancement of glassiness, similarly to what happens in polydisperse systems where a particle-size distribution slows down crystallization. We also characterize avalanches, determining whether their nature within a glass is affected by polydispersity.

Colloids in External Fields

chair W. C. K. Poon

Charging of nanoporous carbon electrodes: The molecular origin of supercapacitance

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Lightweight, low-cost supercapacitors with the capability of rapidly storing a large amount of electrical energy can contribute to meeting continuous energy demands and effectively levelling the cyclic nature of renewable energy sources. The excellent electrochemical performance of supercapacitors is due to a reversible ion adsorption in porous carbon electrodes. Recently, it was demonstrated that ions from the electrolyte could enter subnanometre pores, greatly increasing the capacitance [1]. However, the molecular mechanism of this enhancement remains poorly understood. Using molecular simulations, we have provided the first quantitative picture of the structure of an ionic liquid adsorbed inside realistically modeled microporous carbon electrodes [2]. In this talk, I will show how the separation of the positive and negative ions occurs inside the porous disordered carbons, yielding much higher capacitance values than with simpler electrode geometries. Comparing the charging process at a planar graphite interface with that inside a nanoporous carbon electrode allows us to demonstrate the role of confinement. The proposed mechanism opens the door for the design of materials with improved energy storage capabilities. It also sheds new light on situations where ion adsorption in porous structures or membranes plays a role.

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Phase transition in a 2D colloidal system far from equilibrium

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We use superparamagnetic colloidal particles confined by gravitation to a flat water-air interface as a model system to study the non-equilibrium liquid-solid phase transition in two dimensions. The system temperature is adjustable by changing the strength of an external magnetic field perpendicular to the water-air interface. Increasing the magnetic field on a timescale of ms quenches the liquid to a strongly super-cooled state. If the system is cooled down out of equilibrium the solidification differs drastically from the equilibrium melting and freezing scenario. We did not find any indications of the hexatic phase. The system solidifies to a polycrystalline structures with many grains of different orientation – but our findings do not go along with critical nucleation theory. Shortly after the quench grains are always more likely to shrink and their lifetime is comparable to those of precritical nuclei in the isotropic fluid phase. The local order fluctuates strongly until some grains touch and fluctuations are suppressed. For the early stage, growth exponents and fractal dimensions of the grains are given.

Static and dynamic colloidal organization induced by electrolyte gradients

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We have investigated the self-organization of charged colloids in low salt aqueous solution which occurs, when a large electrolyte releasing object (ERO) is placed in the quasi-2D sedimentation layer next to the like-charged substrate. Two main effects are observed, which strongly depend on the rate of electrolyte release. In either case the gradient in electrolyte (HCl) concentration induces local electric fields due to the grossly different micro-ion mobilities. These fields act on the counterions of the charged substrate and induce radially symmetric flow patterns to or from the electrolyte releasing object, with the direction of flow depending on the charge sign of the wall. For a negatively charged wall a converging flow is observed. For slow rates of electrolyte release particles are swept together at the electrolyte releasing object to form monolayer crystals of triangular lattice. We have been able to map this convergent flow-induced crystallization to a simple model with an attractive potential interaction between ERO and the colloids and quantitatively predict the size-dependent growth velocities and final crystallite size [1]. We anticipate that efficient modeling together with convenient substrate fabrication will facilitate flexibly designing thin crystalline colloidal material of specified microstructure. At large release rates the convergent flow is strong enough to form annular convection rolls, in which the colloids are accumulated and tumbled

about. Instead of crystal formation we observe stationary convection. If in addition EROs are small enough and the loading of the convection cell is asymmetric (e.g. via fluctuations) the whole complex starts to move in a more or less linear fashion with velocities of a few $\mu\text{m/s}$ and macroscopic distances [2]. This self organized self stabilizing emergence of object motion may be regarded as an alternative approach to swimming and transport at low Reynolds numbers.

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Liquid-Crystal Colloid Dispersions I

chair N. M. Silvestre

Nematic colloids: Topology and photonics

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Topology has long been considered as an abstract mathematical discipline with little connection to materials science. However, the emergence of a new class of topological materials provides strong evidence that topology might play an important role in the design of novel materials with counterintuitive properties. The aim of this lecture is twofold. First, we review and discuss the assembly of nematic colloids, where the topological-defect-mediated colloidal interactions are responsible for the striking appearance of the in 2D and 3D nematic colloidal crystals of various symmetries. Here, the singular-point defects in the form of “hedgehogs” play a role that is similar to electric charges. We discuss new experiments that investigate the law of conservation of the topological charge in a novel geometry that allows for the controlled creation and annihilation of topological charges. We demonstrate that by far the most complex are the colloidal interactions mediated by the entanglement of the closed defect loops, where the ultimate topological complexity is demonstrated in knotted and linked chiral nematic colloids [1, 2]. Here, the topological defect loops form knots and links of arbitrary complexity, and are spanned on a colloidal framework. In all cases, the binding energy on nematic colloids is of the order of several $1000 k_B T$. This is several orders of magnitude higher than the interaction of water-based colloids and could provide new strategies for topological soft materials and new applications in photonics. With respect to the second aim, we shall review the recent developments in a novel class of liquid-crystal photonic microdevices: Cholesteric 3D microlasers [3] and electrically tunable nematic microresonators [4]. It will be demonstrated that photonic microdevices made of soft matter outperform their solid-state analogues in many aspects. They have perfect geometrical shapes that

are self-formed by the action of the surface tension, they are mobile, and they can interact strongly and self-organize. We shall demonstrate how simple liquid-crystal photonic microdevices could be assembled by colloidal interactions and we show an example of resonant light transfer from a planar optical waveguide to a tunable nematic microresonator. The future development of liquid crystal photonic microdevices is proposed, such as entangled microphotonic devices realized in double nematic emulsions, colloids on microstructured surfaces and knotted colloidal soft matter.

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Connectedness percolation in complex colloid mixtures

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We present a generalised connectedness-percolation theory for fluid dispersions of mixtures of a large class of colloidal particle that interact via hard-core volume exclusion. Even if we allow for an infinite number of components in the mixture, we are able to derive a compact yet exact expression for the mean cluster size of in some sense connected particles in terms of connectedness direct correlation functions. By invoking an approximate description of the latter, we apply our theory to mixtures of (i) rod-like particles of different dimensions, (ii) plate-like particles, (iii) rod- and plate-like particles and (iv) spherical and rod-like particles. It turns out that mixing colloidal particles of different size and/or shape introduces competing length scales in the dispersion that strongly influence the formation of system-spanning networks that in practical situations are needed, e.g. to produce electrically conductive composites. The interplay between the spatial and angular correlations between different species of particle leads to synergetic or antagonistic percolation, depending on the ease of charge transport between them that in the theory is described by a maximum separation between neighbouring particles in a cluster. This means that the critical concentration of particles needed to form a system-spanning network in a binary mixture can be lower or higher than that of either component. For instance, binary mixtures of disk-like particles of different aspect ratio but the same connectedness range have a percolation threshold that is always lower than that of monodisperse disks, irrespective of their aspect ratio.

Self-organization process in meniscus of smectic-C free-standing films

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In the recent decade, investigations of pattern formation and self-organization of inclusions in liquid crystal free standing films have been the subject of intensive experimental and theoretical investigations. In such liquid crystal free standing films, the spreading of micrometric liquid or solid inclusions induces a subsequent interface deformation around the inclusions: The so-called corona pattern. Nevertheless, up to now, the physical origin of the radial stripes pattern visible in the meniscus surrounding the inclusion remains misunderstood. We investigate extensively the corona pattern using an interferometric technique (phase shifting interferometry [1]) combined with polarised and depolarised optical microscopy. Our interferograms reveal without ambiguity that the radial stripe patterns observed in the smectic-C (or smectic-C*) meniscus correspond to an undulation of the LC-air interface (amplitude ranging from 30 to 100 nm) and was not only originating from surface-induced spontaneous splay [2, 3]. In the thicker part of the meniscus, the undulations propagate themselves in two orthogonal directions and surface exhibits an “egg-box-like” structure. In order to confirm these optical results, we perform an AFM investigation of free-standing films meniscus in the smectic-C phase:

These pictures of the LC-air interface also reveal a periodic undulation of the smectic layers (amplitude ranging from 30 to 100 nm according to places in good agreement with interferometric technique). Lastly, a very basic theoretical model based on the well-known dilatation induced instability [4, 5] is developed and turns out to be compatible with our results for it gives correct orders of magnitude of the undulations wavelengths. From this model, we discuss the physical origin of the corona pattern.

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Active Colloids II

chair U. Jonas

Active motion under external fields and in confinement

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Active motion of microorganisms or artificial microswimmers, such as active colloids, is an appealing subject which has attracted much attention recently. Since these swimmers move constantly in non-equilibrium, they give rise to novel phenomena which, in particular, occur when external fields are applied. The talk reviews our recent work on how active Brownian particles behave in external fields and in confinement. For example, they develop orientational order in a gravitational field [1] and exhibit an interesting instability in dense suspensions when they are bottom-heavy, or they create active fluid pumps in a harmonic trap. Finally, under Poiseuille flow they show nonlinear dynamics reminiscent of the nonlinear pendulum where the bounding walls introduce “dissipation” [2].

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Back to front and upside down: Reversible motion and gravitaxis in simple catalytic swimmers

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We show that a well-known catalytic swimmer – a half platinum coated colloid in hydrogen peroxide – can be made to swim either towards or away from its coated half depending on the concentration of charged surfactants in solution, and that the speed of this motion can be controlled by salt. We use these results to demonstrate that the propulsion mechanism of these particles, previously believed to be based on excluded volume interactions between oxygen and the particle surface, is electrostatic in origin. This has implications for the design of new swimmers, particularly for their potential to function in high salt (i.e. physiological) environments. The direction of motion of these particles also appears to depend upon the angular coverage of the platinum coating, and we explain this by modelling the autophoretic motion of a sphere with non-uniform slip velocity. This presents a potential method for preparing tunable mixtures of spherical pushers and pullers, an ideal model system for studying non-equilibrium phase behaviour. Finally, the heavy platinum coating on these same particles gives them a gravitational torque, causing upwards or downwards motion depending on particle polarity. This gravitational torque can be coupled with a torque arising from deliberate non-uniformities in the platinum coating to produce gravitationally oriented helical trajectories reminiscent of those of gravitactic organisms such as algae.

Autonomous motility and beating in semi-flexible active filaments

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Cilia and flagella are bundles of inextensible elastic filaments that oscillate when forced by the energy transduction of molecular motors controlled and regulated by a chemo-mechanical pacemaker machinery. Experiments on bio-mimicking systems and recent experiments on synthetic active filaments, however, indicate that the pacemaker mechanism is not essential for autonomous motion of these filaments. Here we show, using a Stokesian hydrodynamics description of an elastic filament with a permanent distribution of stresslets along its contour, that the competition between the destabilising effect of hydrodynamic interactions induced by force-free and torque-free active flows, and the stabilising effect of nonlinear elasticity, provides a generic route to spontaneous oscillations and propulsion in these filaments. We show that an initially straight filament is linearly unstable and this instability leads to autonomous filament motion which, depending on conformational symmetry can be translational or rotational. When clamped at one end, the filament develops oscillations, reminiscent of prokaryotic and eukaryotic flagellar motion, now without any period-regulating mechanism.

Self-Assembly II

chair G. Kahl

Electric- and magnetic-field assembly of Janus and patchy particles

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Anisotropically surface modified particles, so-called patchy particles, have been recognized as important building blocks in the directed assembly of particles into desired target structures. Various methods employing shadow evaporation and templating have been used to create spherical particles with anchor patches of controllable size and position. Subsequently, patchy particles can be directed to assemble into interesting structures using electrical and magnetic fields or can be linked chemically via molecular modification of the patches. In this talk, we will report on the preparation of patchy particles using a combination of templates and glancing angle vapor deposition developed in our group. Simple geometrical models are used to predict the patch geometry and relative orientation of the patches. We will further report on the use of patch geometry, material, and position for the pre-programmed, field-directed assembly of such patchy particles in electric and magnetic fields and the potential application of these patchy particles in the assembly of new materials and rheological applications.

Telechelic star polymers as self-assembling units from the molecular to the macroscopic scale

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By means of multiscale molecular simulations, we show that telechelic-star polymers are a simple, robust, and tunable system, which hierarchically self-assembles into soft-patchy particles and mechanically stabilizes selected, open crystalline structures [1]. The self-aggregating patchy behavior can be fully controlled by the number of arms per star and by the fraction of attractive monomeric units at the free ends of the arms. Such self-assembled soft-patchy particles while forming, upon augmenting density, gel-like percolating networks, preserve properties as particle size, number, and arrangement of patches per particle. In particular, we demonstrate that the flexibility inherent in the soft-patchy particles brings forward a novel mechanism that leads to the mechanical stability of diamond and simple cubic crystals over a wide range of densities, and for molecular sizes ranging from about 10 nm up to the micrometer scale.

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Stability, growth, and dynamics of colloidal quasicrystals

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Quasicrystals are non-periodic solids which nevertheless possess long-range positional and orientational order. To obtain colloidal quasicrystals, usually either an external substrate or a pair interaction with at least two characteristic length scales is needed. We study colloidal quasicrystals in order to explore the stability, growth, and dynamics of quasicrystals. For example, by analyzing 2D colloidal quasicrystals that are induced by laser fields with decagonal or tetradecagonal symmetry we obtain new insights into the question why many five-fold symmetric quasicrystals have been identified in nature while not a single quasicrystal with seven-fold symmetry has been observed so far [1]. Furthermore, we study the growth of 3D quasicrystals on substrates. The consequences of defects on the quasicrystalline order are demonstrated. Finally, the dynamics of the colloids due to phasons is explored. Phasons are unique to quasicrystals. Like phonons they are hydrodynamic modes since they do not increase the free energy in the long wavelength limit. The properties of phasons are still intensively discussed in the field. For colloidal quasicrystals, the trajectories of colloidal particles due to a phasonic drift can be obtained by simulations or determined theoretically [2]. These observations help to get a deeper insight into the properties of phasonic displacements in colloidal as well as in atomic quasicrystals.

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Arrested States II

chair P. S. Clegg

Multiple arrested states in a charged colloidal system

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Dynamical arrest in colloidal and, more generally, in soft matter systems, has recently become the subject of intense research activity also because of its theoretical and technological implications. It is well known, in fact, that colloidal systems are very good models for understanding the general problem of dynamic arrest, showing a larger flexibility compared to atomic and molecular glasses. The fine tuning of the control parameters opens the possibility to tailor the macroscopic properties of the resulting nonergodic states. Several mechanisms of dynamical arrest have been identified. Few real systems are suitable for use as experimental counterparts for the vivid theoretical speculations on non-linear, complex and non-equilibrium systems. Among these colloidal clays have emerged as suitable candidates to investigate the formation of multiple arrested states. In this presentation we show the results obtained on dilute suspensions of laponite, an industrial synthetic clay. Once dispersed in water laponite originates a charged colloidal system of nanometer-sized discotic platelets with inhomogeneous charge distribution and directional interactions. The presence of competing attractive and repulsive terms in the interactions, combined with the anisotropy of the face-rim charge interactions and with the discotic shape of laponite, produce a very rich phase diagram including a nontrivial aging dynamics towards multiple arrested states. We focus here on two different disordered arrested states of gel and glass, obtained respectively for low ($C_w < 2.0\%$) and high ($C_w \geq 2.0\%$) clay concentrations in salt free water conditions. The arrested state at low concentration is governed by attractive

interactions and experimental findings supported by numerical simulations have recently furnished the first experimental evidence of empty liquid and equilibrium gel, respectively found for ($C_w < 1.0\%$) and ($1.0\% < C_w < 2.0\%$) [1]. These new concepts were formulated for patchy colloids [2] of different shapes, patterns and functionalities that are considered the novel building blocks of a bottom-up approach toward the realization of self-assembled bulk materials with pre-defined properties. On the other side the comparison between dynamic light scattering, small angle X-ray scattering and dilution experiments with theoretical and numerical results have permitted to individuate an high concentration ($C_w \geq 2.0\%$) Wigner glass [3] state, i.e. an arrested state formed by disconnected particles or clusters and stabilized by the electrostatic repulsion. Moreover very recent results show that the attractive interactions are playing a role also in this case and that even in the glassy state the local structures and the interactions among the colloidal particles are still evolving, originating a dichotomic behaviour [4].

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Soft colloids with tunable interactions – microgels as models for soft dipolar fluids

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Cross-linked poly(N-isopropylacrylamide) (PNIPAM) microgel particles constitute an interesting class of colloidal systems which possess a variable degree of softness and a tuneable interaction potential. This can be varied between hard sphere and very soft repulsive [1]. We use monodisperse neutral and ionic PNIPAM microgels as model systems for soft repulsive colloids, where we tune the interaction potential from long-range Yukawa-like at large distances to a much softer repulsive interaction (Hertzian type) at short distances [2, 3]. The anisotropic (dipolar) contribution to the soft repulsive interaction potential can be tuned with an external electric field [4]. We study the density dependent structural ordering and concomitant phase transitions in situ with confocal laser scanning microscopy (CLSM) at effective volume fractions Φ_{eff} below and above close packing volume fraction Φ_{cp} . For neutral microgels interacting with a Hertzian repulsive potential, we find fluid-crystal and fluid-glass transitions. Moreover, the density dependent pair correlation function $g(r)$ clearly exhibits anomalies at Φ_{eff} beyond glass transition volume fraction ($= 0.65$) which we interpret as a structural signature of the glass transition related to the particle softness [2]. In the case of ionic microgels in an

external electric field, we find various field-induced structural transitions below and above close packing [4]. At low $\Phi_{eff} < \Phi_{cp}$ we observe a transition from an isotropic to a string fluid. At $\Phi_{eff} = 0.85$, there is a reversible transition from an amorphous to a dipolar crystalline state, followed by the onset of a gas-(string) solid coexistence. At $\Phi_{eff} = 1.6$ and 2.0 , i.e. far above close packing, evidence for a field-induced arrested phase separation is found. These results are discussed in light of the previously studied phase behavior of colloidal systems interacting with hard and soft repulsive interaction potentials.

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Probing dynamics of hard sphere suspensions at high volume fractions with coherent X-rays

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Colloidal suspensions of spherical particles presenting hard-sphere like interactions is one of the simplest and most widely studied systems of soft condensed matter. They can be treated as a model for testing fundamental theories regarding e.g. crystallization [1] or glass transition [2]. Despite the long history of both theoretical and experimental research, the dynamic behavior of hard sphere suspensions still lacks a complete understanding. X-ray photon correlation spectroscopy is a coherent scattering technique equivalent to dynamic light scattering (DLS) [3], which is one of the main tools used in the study of colloidal dynamics [4]. Comparing to visible light, the use of X rays provides access to higher momentum transfer vector values and allows to avoid multiple scattering – a phenomenon significantly complicating DLS measurements on concentrated samples. Moreover, the use of a fast, single photon counting area detector available at the ID10 beamline at ESRF gives insight into the evolution of sample dynamics during the measurement time by the means of two-time correlation functions. In this work suspensions of sterically stabilized poly(methyl methacrylate) colloidal spheres were used. Particle size, polydispersity and concentrations of the samples were obtained using the small-angle X-ray scattering technique. The probed volume fractions extend above the putative mode coupling theory glass transition concentration of 0.57. Unexpectedly, instead of freezing out

of equilibrium with divergent relaxation times, the system preserves ergodicity at the highest probed volume fraction of nearly 0.6. The relaxation rates are well described by functional forms suggesting that the slowing-down is governed rather by jamming than glass transition, occurring at higher packing fractions. Similar behaviour has been recently reported by Brambilla et al. in Ref. [5], where the authors used DLS to probe the dynamics. Additionally, the generalized Stokes-Einstein relation [6] has been used to probe the frequency-dependent linear viscoelastic moduli of the samples, revealing a transition from liquid- to solid-like response upon increase of concentration. This is accompanied by the emergence of “anomalous dynamics”, characterized by faster-than-exponential relaxation rates, ballistic dispersion relationships, and strong heterogeneities.

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Active Colloids III

chair D. Frenkel

Emergent dynamics and self-assembly in field driven active colloids

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Ensembles of interacting colloidal particles subject to an external periodic forcing often develop nontrivial collective behavior. External fields provide us with an effective tool to drive colloidal ensembles out of equilibrium and control interaction profiles of colloids. I will present nontrivial emergent phenomena in magnetic colloidal ensembles suspended at liquid-liquid or liquid-air interfaces and driven out of equilibrium by uniaxial alternating magnetic fields. Experiments reveal new types of nontrivially ordered dynamic self-assembled structures (in particular, “asters”, “snakes”) emerging in such systems in a certain range of excitation parameters. Transitions between different self-assembled phases with parameters of external driving magnetic field are observed. Above certain frequency threshold dynamic self-assembled structures can spontaneously break the symmetry of self-induced surface flows (symmetry breaking instability) and turn into swimmers. Induced self-propulsion of robust aster-like structures in a presence of small in-plane DC field perturbations has been discovered. A possibility of the directed cargo transport at the interface by self-assembled structures is demonstrated. Unusual magnetic ordering is discussed. Some features of the self-localized structures can be understood in the framework of an amplitude equation for parametric waves coupled to the conservation law equation describing the evolution of the magnetic particle density. Molecular dynamic simulations capturing microscopic mechanisms of the non-equilibrium self-assembly in these out-of-equilibrium systems are presented. The research was supported by the U. S. DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under the Contract No. DE AC02-06CH11357.

The unexpected behaviour of swimming-cells systems under the influence of external force fields

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Systems composed by self-propelled individuals, such as swimming bacteria, may display a surprising behaviour when compared to thermally equilibrated colloidal systems. Unexpected situations emerge in particular when these systems are subject to some external perturbation. It was indeed shown that artificial microstructures can rectify the motion of bacteria interacting with them [1]. Moreover adequately designed microobjects can be driven unidirectionally by motile cells [2]. Recently it was also demonstrated that novel interaction mechanisms emerge between artificial particle surrounded by swimming bacteria [3]. These intriguing phenomena have made “active matter” a subject of profound interest for physicists since, in most of these cases, the interplay between the dynamics of the self propelled particles and the imposed external perturbation leads to a behaviour that substantially differs from that of inanimate matter. In this presentation I will review these results from a statistical-mechanics perspective introducing a number of novel theoretical tools for describing the properties of these active systems when perturbations are considered. Moreover I will present new experimental results regarding the dynamics of bacteria under the action of a centrifugal acceleration [4]. This experiment demonstrates that high-motility bacteria can be efficiently selected by the application of a simple centrifugal field. Such observations underline the significant heterogeneity of the motility among the bacteria population and suggest important details to be considered in modelling the dynamics of swimming cells.

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Emergent structures of active colloid suspensions under gravity

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The sedimentation process in a suspension of bacteria is the result of the competition of gravity and the intrinsic motion of the microorganisms. I will discuss the outcome of coarse-grained numerical simulations of run-and-tumble squirmer suspensions studying the variation of the non-equilibrium steady state as a function of the interplay between squirmers' swimming speed and gravity. For high enough bacterial activity, the density profiles characterizing the squirmer sediment are no longer simple exponentials. The observed sediments can be understood in some cases in terms of a local effective temperature, suggesting that the break-down of the exponential form is a collective effect due to the onset of fluid-mediated dynamic correlations among particles. I will contrast this behavior with the patterns formed by a suspension of active colloids under the action of gravity, when their intrinsic motion emerges from inhomogeneous surface reactions. We analyze the role of the hydrodynamic coupling in the patterns these suspensions develop and the role that the hydrodynamic coupling plays in this case.

Applications

chair F. G. Lo Verso

Application of complex colloids in fast moving consumer goods

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Designed colloids find application in many technologies and in the processing of various materials. In fast moving consumer goods such as food, personal care and home care products colloids, are either naturally present, formed during the processing, or intentionally added to tailor certain functional properties of the product. In this talk, we will discuss the fundamental approaches and recent developments in the area of using designed colloids to control product functionality such as composition, microstructure, texture, stability, appearance, and the biophysical aspect of taste, delivery and digestion of nutrients and other functional ingredients.

Microfluidics: A nice tool to study oil enhanced recovery processes

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An important class of “out-of-equilibrium” patterns occurs by forcing immiscible fluids in interconnected thin gap networks, a phenomenon frequently encountered in nature as well as in many manmade systems. Illustrative examples include mineral processing, painting, construction engineering, printing, oil recovery, and soil mechanics. These fluid-fluid or fluid-gas displacements generate preferential flow pathways along one of the fluid flows, forming patterns ranging from compact to ramified and fractal. The formation and selection of these patterns are challenging problems in the field of nonequilibrium physics and central for many industrial applications. One of the major difficulties in achieving a good understanding of preferential pathways in interconnected network is the large number of parameters potentially involved. These include the viscosity of the two fluids, the surface tension between them, the wetting properties, their respective flow rates, the topology of the network, and the considered length scales. These phenomena were experimentally evidenced using micromodels of porous media which allow direct observations of the phases displacements. However, at this stage, the comparison between experiments and theory remains usually qualitative or semiquantitative and is limited to the features of the patterns. Microfluidic techniques offer the opportunity to fabricate micromodels with well-defined surface and geometrical features. In this work, we revisit this problem using these to fabricate networks of straight microchannels with controlled size heterogeneities. Great care is brought to the control of the wetting properties. The features of the flow are determined from the movies of the filling of the micromodel. The measurement of the

local velocities is compared to numerical simulations based on a network model where the exact geometrical features of the micromodels are incorporated. We will discuss the situation of water wet rocks as well as oil wet ones. In the last part of the talk, we will deal with the flow of non-Newtonian fluids. We will show that they are less efficient than Newtonian ones to recover oil.

Liquid-crystalline nanomicelles for active drug delivery system

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Based on the amphiphilic diblock copolymer for drug delivery system (DDS), we have designed a liquid crystal nanomicelle water solution made from the PEG-side chain liquid crystal diblock copolymers. Mesogenic hydrophobic part of diblock copolymers form can form a liquid-crystalline (LC) state in the tiny nanomicelles dispersed in the water by the hydrophilic PEG part. However, although each nanomicelle locally have anisotropy, nanomicelle water solution never show the microscopic anisotropy, because they are freely rotating in the water solution and each anisotropy is completely randomized in much larger scale. Here, we have experimentally confirmed the existence of the LC state in the tiny nanomicelles by the depolarized dynamic light scattering. Detailed analysis of the dispersion relation of the hydrodynamic modes clarified the dynamics of the LC nanomicelles and space dependent dynamics of the director fluctuation in the nanocarrier. From the temperature dependence of the fast VH mode, phase transition between LC and liquid state confined in the tiny isolated shells looks continuous on the contrary to the weak first order transition in the bulk isotropic nematic phase transition. Namely, wave number dependence of the fluctuation modes clearly visualizes the space heterogeneity of the random self-organized system with a lack of the regularity whereas the static investigation such as microscopy and scattering is completely useless for every scale from visible light to X rays. Thus, we have designed prototype LC nanomicelle for the active DDS system to control the holding and releasing the drug by the liquid-

liquid crystal-solid phase transition. In turn, it is interesting that the phase transition phenomena confined in the tiny isolated space on the view point of the statistical physics by changing the size of the micelle. Since the model LC diblock polymer contains the azo dye in the mesogenic part, it is also possible to excite the phase transition by shining the strong laser dye.

Rheology II

chair S. Kantorovich

Ageing and flow instability in soft glassy materials

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We review recent theoretical progress in modeling the rheology and aging of soft glassy materials. Particular attention will be paid to the issue of flow instabilities such as shear banding, and their interaction with the underlying ageing dynamics of these materials.

Nonlinear coupling in biaxially sheared dense colloidal suspensions

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When a physical system is slightly perturbed with two different frequencies in the linear regime, the response of these two modes are independent. However, when one mode increases in strength and brings the system far away from equilibrium, a coupling between the two modes can emerge, which reveals the nature of nonlinear interactions in the system and can be used effectively to manipulate out-of-equilibrium material properties. Here, we investigate the out-of-equilibrium mode couplings in colloidal suspensions under biaxial shear. We impose two different shear frequencies to a dense colloidal suspension and measure the corresponding stress spectra with a novel 2D force measurement device. We observe a strong enhancement in the viscosity of the lower frequency (primary) mode when the shear rate of the higher frequency (secondary) mode is large. This change in viscosity also depends on the relative orientation between the two modes – the coupling is even more pronounced when the secondary flow is orthogonal to the primary flow. Using confocal microscopy, we also image the structure of the suspensions and study the microscopic origin of this response coupling.

Simulations of colloids in active fluids: Negative drag and aggregation properties

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Active fluids are suspensions of particles that use their own energy in order to do work. Examples can be found mainly, even though not solely, in biological contexts. Examples are bacterial or algae suspensions, and the actomyosin solution. These out-of-equilibrium materials show a range of novel properties that in large extent still are to be investigated. As it is currently done in soft matter physics, one could think of using colloids as probes to investigate the behaviour of active fluids at the micron scale. I will present simulations of microrheology experiments in active fluids which show a behaviour in striking contrast with the one of their passive analogue. In particular, we define an effective viscosity, according to Stokes law, and find an important dependence on the probe size [1, 2] and a region of instability characterised by a steady state of negative drag [2]. Moreover, I will present an initial study on the aggregation of many colloids in active materials.

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Liquid-Crystal Colloid Dispersions II

chair P. Cluzeau

The isotropic-to-nematic phase transition in hard helices: Onsager-like theory and Monte Carlo simulation

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The helix is a typical structural motif in nature: For example, polynucleotides, proteins and collagen fibres are all right-handed helices. Rigid and semiflexible helical polymers can exhibit ordered phases, whose features are only partially understood. We have investigated the isotropic-to-nematic phase transition in systems of hard helical particles, using Onsager theory and Monte Carlo computer simulations. Motivation of this work resides in the ubiquity of the helical shape motif in many natural and synthetic polymers, as well as in the well known importance that the details of size and shape have in determining the phase behaviour and properties of soft condensed matter systems. We discuss the differences with the corresponding spherocylinder phase diagram and find that the helix parameters affect the phase behaviour and the existence of the nematic phase. Onsager theory predicts the nematic-isotropic transition at higher density with increasing helicity. We find that at high helicities Onsager theory significantly departs from numerical simulations even when a Parsons-Lee improvement is included to account for the non-convexity of particles. When compared to the Monte Carlo simulation data, Onsager theory generally underestimates pressure, with the deviations

increasing with increasing density and upon going from the isotropic to the nematic phase. The unexplored compact structure realm occurring for such non-convex objects at high densities and pressures will also be briefly discussed.

Using partially miscible solvents to control colloidal stability and the assembly of colloidal rods

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In our experimental study we investigate three-component systems consisting of colloidal particles in a partially miscible binary liquid mixture. The colloids are charge stabilized in the separate liquids, and in the phase-separated liquid mixture they are confined into one of the phases, demonstrating complete wetting by this (colloid-preferred) component. First, we show that these systems often exhibit partial aggregation, leaving a fraction of the colloids stable in the supernatant, as the binodal of the liquid mixture is approached parallel to the liquid composition axis. Compared to previous observations in similar systems [1], the aggregation behaviour is different and sets in much further from the liquid-liquid binodal. The effect involves adsorption of this component onto particles, eventually leading to capillary condensation as adsorbed layers meet. Second, we use a system where aggregation only occurs very close to the liquid-liquid binodal, and set the liquid composition poor in colloid-preferred component to confine colloidal rods [2] into a small volume by a rapid temperature quench into the two-fluid region. This way the rods are forced to assemble into (ordered) liquid crystalline phases (nematic and smectic) or into (disordered) percolating networks.

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Modeling the assembly of colloids with sharp features in nematic liquid crystals

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The self-assembly of colloids in nematic liquid crystals via topological defects has been extensively studied for spherical particles, and some investigations have considered the role of particle anisotropy. Recent advances in microfabrication techniques have led to homeotropic-aligning colloids with more complex shapes, such as cylinders and “microbullets”, which contain sharp corners. We use Landau-de Gennes numerical modeling to investigate the nematic director field and defect structure around such colloids in a thin-cell geometry, and we determine the colloids' equilibrium alignment directions and effective pair interaction potentials as a function of a few relevant shape parameters. We find that small-scale features of complex colloids have significant effects on defect structure and colloidal assembly in ways not captured by far-field approximations. This raises the possibility of selecting self-assembled colloidal structures by tuning particle shape.

Self-Assembly III

chair A. Šiber

Inverse patchy colloids: Effect of the interplay between attractive and repulsive anisotropic interactions on the collective behaviours

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Over the past decade, the already vast possibilities offered by colloidal particles as building blocks for new materials have been substantially widened by the advent of patchy colloids, i.e. colloidal particles with chemically or physically patterned surfaces. By virtue of the well-defined bonding geometries, patchy particles are nowadays regarded as ideal units of novel self-assembled materials with specific symmetries and physical properties. We have recently introduced a new class of patchy particles, which we refer to as inverse patchy colloids (IPCs). While patchy systems are typically characterized by the presence of attractive regions on the surface of otherwise repulsive particles, IPCs are mutually repulsive particles carrying extended patches that repel each other and attract those parts of the colloid that are free of patches. Examples of IPCs are colloidal particles with a heterogeneous surface charge distribution. We have developed a suitable description of such systems starting from first principles in order to keep a connection with the microscopic systems. The main feature of IPC systems is not anymore the limited valence in bonding, but rather a competitive interplay between attractive and repulsive anisotropic interactions. The role of such an interplay as well as the effect of the patch extension have been studied with respect to collective phenomena such as crystal formation, dynamical arrest or the gas-liquid phase separation. The investigation of a wide selection of IPC systems in the bulk as well as in a confined geometry, together with the study of the two-dimensional counterparts of such systems, gave evidence of very promising self-assembly scenarios, such as planar and even ordered porous structures.

Computer simulations of attractive one-patch colloids

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The surface of colloids can be chemically modified to create attractive patches that allow for directional interactions [1, 2]. The resulting “patchy colloids” [3] are very useful as model systems. In computer simulations, the essential physics can be captured using patchy particles with only a simple Kern-Frenkel square-well attraction [4]. Interestingly, already the simplest patchy architectures result in intriguing and exotic phase behaviour. For example, Janus spheres [5, 6] with one attractive hemisphere can form clusters, micelles, curved bilayer sheets, and various crystals [7, 8]. Amongst all these structures, the interplay between the interaction range and the patch size is crucial. Here, we give an overview of structures that were found for one-patch colloids. In the case of spherical colloids with a low patch-surface coverage (30%) but relatively long interaction ranges of half the particle diameter, we discovered the formation of long wires instead of the clusters and micelles that were found at the lowest coverage fractions [9]. For a higher coverage fraction (40%), bilayer sheets appeared. In studying the thermodynamic properties of structures percolating in one or two dimensions, we encountered unexpected theoretical problems that were previously unnoticed. We deal with those in calculating the stability of the wires and bilayer sheets. In the case of Janus colloids, bilayer sheets can compete and coexist with both the fluid and crystal phases. For non-spherical one-patch colloids, micelles and bilayers can form as well: Dumbbells

consisting of a partially overlapping attractive sphere and a non-attractive sphere can form extended sheets that fold into large micelles.

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Valency without patches: Many-body effects in DNA-coated colloids

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DNA-coated colloids are promising building blocks for guiding self-assembly at the mesoscopic scale. Recently, we have introduced an accurate and general self-consistent theory for the effective free energy of interaction of a set of such colloids, one that fully captures competitive and many-body effects. Here, we show how one kind of many-body effect that arises when the DNA linkers on these colloids are mobile, a possibility that has recently been realized experimentally. Such effects may be used to endow isotropic spherical particles with valency, that is, the ability for this particle to have a coordination number below that implied by packing considerations. Such control, traditionally implemented by decorating the particles with particular geometric arrangements of small patches, is expected to allow open structures of colloidal particles to be assembled. We discuss the phase behaviour and assembly kinetics of this new kind of DNA-coated colloids and the possible technological applications that they enable.

Posters

Ordered structures in confined soft particle systems

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We identify the emerging sequence of ordered equilibrium structures of soft particles confined in a slab geometry as the slab width grows, starting from a two-dimensional lattice. The energetically most favorable structures are determined using an optimization tool based on genetic algorithms. Apart from multilayer structures that show triangular and square symmetry, we observe intermediate structures that differ substantially from the ones observed in hard spheres systems; moreover, there is evidence that those intermediate crystal phases depend in our slab geometry on the softness of the interaction potential. We identify and verify a scaling law for the ground-state energy and structure of the system. We investigate the thermal stability of the intermediate phases using Monte Carlo simulations under the same external constraints. While some structures remain stable for sufficiently low temperatures, we find evidence that this does not hold for more complex structures. Using multi-histogram reweighting, we find excellent agreement between the zero-temperature ground state calculations and the finite-temperature Monte Carlo simulations carried out at relatively low temperatures.

Charged colloidal system in the monoclonal antibody phase behavior

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Colloidal interactions between proteins determine the phase behavior, stability and cluster formation propensity of globular proteins, such as monoclonal antibodies, in an electrolyte solution. To study these events, we experimentally determined intermolecular interactions in dilute protein solutions via the second virial coefficient, in order to understand protein-protein interactions and protein phase behavior. The repulsive electrostatic part of the Derjaguin–Landau–Verwey–Overbeek (DLVO) interaction model for a spherical protein was quantified via the homogeneously smeared protein surface charge and/or surface potential over the spherical protein surfaces. The attractive van der Waals interactions part was quantified via their Hamaker coefficient, both as a function of ionic strength and pH of the bathing solution. In addition, a steric barrier in the form of a “hydration layer” is sometimes assumed to surround the molecules and effectively represents an additional excluded volume term [1, 2]. We evaluate the extracted parameters of DLVO interactions and assess the overall applicability of this model to mAbs interactions in view of the fact that it does not consider any ion specificity, protein solvation/hydration and protein anisotropy.

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Rotation control of microscopic oblate particles by light vortex beams

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Many recent works have pointed out the importance of the asymmetry of colloidal particles in their dynamics properties when these are subjected to an external field. In this work we studied the induced rotation of oblate particles by the angular momentum of an elliptically polarized vortex beam. We used polystyrene oblate particles of about 2 μm in size and aspect ratios between 0.5 and 1. We showed experimentally that these particles can be confined in 3D by a light beam, and at the same time can be rotated by a torque that depends on the shape of the particles and vorticity of the beam. Moreover, we demonstrate in a more general case that the particle dynamics can be described by three components of the rotation of a rigid body: Spin, precession and nutation. Using an optically addressed spatial light modulator, we were able to rotate more than one particle at a time and control their frequency and sense of rotation independently. These results provide a simple approach to generate or study fluid flows and hydrodynamic interactions in the microscopic realm, as an alternative to the former techniques based on birefringent, absorbent or chiral particles.

Phase diagram of soft disks

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The ordered phases of many nanocolloidal particles such as dendrimer and diblock copolymer micelles are characterized by open rather than close-packed lattices [1], their phase diagram typically being far richer than in classical colloids. The origin of the open packings is presently still unknown and it could be related to the deformability of the nanocolloids [2, 3]. Here we model the nanocolloids as homogeneous solid particles described by classical theory of isotropic elasticity. Using both Hookean and neo-Hookean models, we study the stability of regular 2D lattices of monodisperse elastic disks. The shape and the energy of disks in the columnar, honeycomb, square, and hexagonal lattice is computed using the finite-element method implemented in the open-source freeFEM++ package [4]. We construct the phase diagram in the (density, Poisson ratio)-plane and we discuss possible implications of our theory for 3D soft particles.

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The existence of soft cluster crystals

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We perform extensive monomer-resolved computer simulations of suitably designed amphiphilic dendritic macromolecules over a broad range of densities, proving the existence and stability of cluster crystals formed in these systems, as predicted previously on the basis of effective pair potentials [1]. Key properties of these crystals, such as the adjustment of their site occupancy with density and the possibility to heal defects by dendrimer migration, are confirmed on the monomer-resolved picture. At the same time, important differences from the predictions of the pair potential picture, stemming from steric crowding, arise as well, and they place an upper limit in the density for which such crystals can exist.

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The existence of a bending rigidity for a hard sphere liquid in contact with a large colloidal particle: Helfrich or Hadwiger?

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In the context of Rosenfeld's fundamental measure theory [1, 2], we show that the bending rigidity is not equal to zero for a hard-sphere fluid in contact with a large colloidal particle modeled as a hard curved wall. The implication is that the Hadwiger theorem does not hold in this case [3, 4] and the surface free energy is given by the Helfrich expansion instead [5]. The value obtained for the bending rigidity is (i) an order of magnitude smaller than the bending constant associated with Gaussian curvature, (ii) changes sign as a function of the fluid volume fraction, (iii) is independent of the choice for the location of the hard wall.

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Flexoelectric and order-electric switching between nematic wetting morphologies

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Using hybrid lattice-Boltzmann/finite difference simulations, we model a nematic liquid crystal, in coexistence with its isotropic phase, filling a substrate patterned with rectangular grooves. We analyse its response to an externally-applied electric field, under flexoelectric and order-electric couplings, with an emphasis on identifying switching transitions between bistable morphological states. We identify that order-electricity provides a means of wetting and dewetting the substrate plateaux with a nematic layer, without affecting the configuration of the nematic within the groove. We identify that flexoelectricity is a viable means of changing the topological configuration of the nematic in the groove, provided that the coupling differentiates between the type of distortion at the corners of the substrate. We determine quantitatively the field magnitudes and orientations required to effect each type of transition. We show how flexoelectric textures in the bulk nematic may be used as a means for colloidal self-assembly.

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Pore scale models for imbibition and drainage in etched microfluidic junctions from micromodel experiments and direct lattice-Boltzmann flow calculations

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We investigate both drainage and spontaneous imbibition processes at the pore scale using a combination of microfluidic experiments and lattice-Boltzmann (LB) flow calculations. The application is CO₂ injection in downhole rock formation for carbon storage and enhanced oil recovery. First, we have fabricated a range of specifically designed etched micro-models to investigate the role of pore shape and throat width on fluid displacement. These designs include junctions with both equal and unequal channel widths in order to achieve a range of capillary entry pressures. All models were etched into poly(methyl methacrylate) and chemically treated to create a hydrophobic surface. The displacement process is captured via a high-speed video microscope under ambient conditions. The experimental results were then directly compared with LB simulations. For the drainage experiments, we observe that the fluid displacement in the junction follows the Young-Laplace law. For the case of spontaneous imbibition, however, the models with unequal channel widths display different displacement behaviour. Our experimental observations are confirmed in detail by LB simulations, lending credibility to our observations. Instead of following Young-Laplace filling rules, we observe that the throat in closest proximity fills up first. This has potentially important consequences for calculation of residual saturation of CO₂ at the core scale, which is determined by spontaneous imbibition of brine following CO₂ injection.

Colloidal lattice shearing and rupturing with a driven line of particles

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We examine the dynamics of two-dimensional colloidal systems using numerical simulations of a system with a drive applied to a thin region in the middle of the sample to produce a local shear. For a monodisperse colloidal assembly, we find a well defined decoupling transition separating a regime of elastic motion from a plastic phase where the particles in the driven region break away or decouple from the particles in the bulk, producing a shear band. For a bidisperse assembly, we find that the onset of a bulk disordering transition coincides with the broadening of the shear band. We identify several distinct dynamical regimes that are correlated with features in the velocity-force curves. As a function of bidispersity, the decoupling force shows a nonmonotonic behavior associated with features in the noise fluctuations, power spectra, and bulk velocity profiles. When pinning is added in the bulk, we find that the shear band regions can become more localized, causing a decoupling of the driven particles from the bulk particles. For a system with thermal noise and no pinning, the shear band region becomes more extended and the average velocity of the driven particles drops at the thermal disordering transition of the bulk system.

Collective ordering of colloids in grafted polymer layers

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A grafted polymer layer can be used to prevent the deposition of colloidal particles on a solid surface. We present Monte Carlo and molecular dynamics simulations that show that, under the influence of sufficiently strong external fields, a collective instability allows the colloids to penetrate and form internally ordered, columnar structures that span the polymer layer. The morphology of the patterns that form depends sensitively on the strength of the applied field. Depending on the conditions, the colloidal clusters may be isolated or laterally percolating. Interestingly, external fields are not essential to obtain such colloidal patterns: The same structures can be achieved by compressing a “sandwich” of two grafted polymer layers with (nano)particles in between. Our results suggest a simple method for fabricating polymer films containing layer-spanning, (nano)colloidal structures thus opening up a new route for the design of thin structured films.

Unveiling the complex glassy dynamics of short-range square shoulder systems: Simulations and theory

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Dynamical arrest in soft matter systems has revealed in the last few years a wealth of novel glass states with associated distinctive dynamics. In this work we report results of extensive molecular dynamics (MD) simulations, supplemented by mode coupling theory (MCT) calculations for the square shoulder model, a purely repulsive potential where the hard-core is complemented by a finite shoulder. This model has been used to describe the behavior of some metallic glasses or complex materials like micellar or granular systems as well as primitive model of silica and water. For the one-component version of this model, MCT predicted the presence of diffusion anomalies both upon cooling and upon compression and the occurrence of glass-glass transitions. In the simulations, we focus on a non-crystallizing binary mixture, which, at the investigated shoulder width, shows a non-monotonic behavior of the diffusion upon cooling but not upon isothermal compression. In addition, we find the presence of a disconnected glass-glass line in the phase diagram, ending in two higher-order singularities. These points generate a logarithmic dependence of the density correlators as well as a subdiffusive behavior of the mean squared displacement, although with the interference of the nearby liquid-glass transition. We also perform novel MCT calculations using as input the partial structure factors obtained within MD, confirming the simulation results. The presence of two hard sphere glasses, differing only in their hard core length, is revealed, showing that the simple competition between the two is sufficient for creating a rather complex dynamical behavior. Finally we have detected the

presence of a special locus in the phase diagram occurring at a certain distance to the glass-glass transition where the influence of the liquid-glass boundary does not yet interfere with the glass-glass one. Along this line, the system displays invariant dynamics at all length and time scales.

Bicontinuous and mixed gels in patchy colloidal mixtures

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We investigate the thermodynamics and percolation regimes of model binary mixtures of patchy colloidal particles [1]. The particles of each species have three interaction sites of two types, one of which promotes bonding of particles of the same species while the other promotes bonding of different species. We find up to four percolated structures at low temperatures and densities: Two gels where only one species percolates, a mixed gel where particles of both species percolate but neither species percolates separately, and a bicontinuous gel or bigel where particles of both species percolate separately forming two interconnected networks. The competition between the entropy and the energy of bonding drives the stability of the different percolating structures. Appropriate mixtures exhibit one or more connectivity transitions between the mixed and bicontinuous gels, as the temperature and/or the composition of the mixture changes.

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The stacking diagram of colloidal mixtures under gravity

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Sedimentation of colloids is strongly affected by gravity because their gravitational and thermal energies are comparable. Gravity plays a major role in determining the stacking sequence in a sedimentation equilibrium experiment. We present a theory to describe the relation between the bulk phase diagram of a colloidal mixture and the stacking sequence observed in sedimentation equilibrium experiments. We demonstrate there is a unique and invertible correspondence between the bulk phase diagram and the stacking diagram, i.e. the set of all different stacking sequences under gravity. We apply the theory to predict the stacking diagram of a binary mixture of colloidal platelets.

Liquid crystal ordering by short DNA duplexes self-assembly

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Concentrated solutions of short blunt-ended DNA duplexes, as short as 6 base pairs, are known to order into the nematic liquid crystal phases. This self-assembly is due to the stacking interactions between duplex terminals, which promotes their aggregation into polydisperse chains with a significant persistence length. Experiments show that liquid crystal phases form above a critical volume fraction depending on the duplex length. We investigate two coarse-grained models of DNA double-helical duplexes by means of numerical simulations and a recently proposed theoretical framework. In the first model (SQ) the DNA duplex is represented as a hard quasi-cylinder whose bases are decorated with two identical reactive sites and the stacking interaction between terminal sites is modeled via a short-range square-well potential. In the second model, which is less minimalist, nucleotides are represented as rigid bodies with three interaction sites. We compare numerical results with theoretical predictions and find a satisfactory quantitative matching of the system structure in the isotropic phase for both models. For the SQ model we also find an acceptable agreement between theoretical and numerical results for the isotropic-nematic phase boundaries. Finally the comparison of critical concentrations calculated theoretically for both models with experimental findings enables us to provide an estimate of the coaxial stacking energy in line with experimental expectations.

A lattice-Boltzmann study of semi-permeable colloids

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The role of permeability can be observed in everyday life. Well known examples range from biological and synthetic membranes [1-3] to synthetic vesicles [2] which show great potential in biomedical fields such as drug and gene carriers of therapeutic compounds. We study the electrokinetic response of semi-permeable spherical colloids. In our study semi-permeable colloids are placed in contact with a solution which is composed of cations and anions with equal charge in a solvent. In our application only cations and anions are allowed to permeate through the semi-permeable colloidal shell. The lattice-Boltzmann (LB) technique that we apply is that of Capuani, Pagonabarraga and Frenkel's model which is described in great detail in Ref. [4]. Their model considers fluxes between connected nodes as the basic physical quantities that determine the evolution of local densities which helps overcome some of the limitations of previous LB models [4]. We find that the study of the electrokinetic response is not only interesting from a physical point of view but also practical in biological and synthetic objects.

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Depletion interaction studied by evanescent wave scattering

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TIRM is a versatile tool to measure particle/wall interaction potentials. Purely optical, it is completely non-invasive. Utilizing a probability distribution inversion a potential can be derived from intensity fluctuations caused by Brownian motion. With this technique is possible then to investigate very small forces (with fN precision) like the ones involved in depletion interactions or van der Waals attraction. Here TIRM will be used to study biomimetic systems. In particular the depletion interaction caused by fd viruses at intermediate concentrations, the total interaction between protein coated surfaces and forces between DNA brushes will be investigated.

Diffusive dynamics of colloids in confined flow

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We studied the flow of concentrated hard sphere suspensions through microchannels. Using silica spheres with fluorescent cores allowed visualizing particle motions in real time with a confocal scanning laser microscope. Using an adapted particle tracking algorithm, we could quantify both convective and diffusive motions as a function of particle volume fraction, Péclet number and channel geometry. Up to volume fractions of 0.4, the average flow patterns compare well to calculations for Newtonian fluids in rectangular geometries. Especially the apparent diffusion coefficient near the channel walls shows an interesting behavior: Both at low and at high Péclet numbers, the mean squared displacement perpendicular to the flow direction shows a decrease as the wall is approached. However the physical origins appear to be quite different. Additionally, also microchannels with structured walls were explored. Micrometer-scale corrugations, designed using soft lithography, turned out to be effective in eliminating wall slip. Besides that they also served as pockets, in which the particles diffuse slowly and reside considerably longer, as compared to a smooth wall. They present an interesting case for studying the relation between wall roughness and fouling in microchannels.

Bonded boojum-colloids close to curved surfaces

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

Bridge function and static structure of the one-patch Kern-Frenkel model

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The exact bridge function of the short-range anisotropic one-patch Kern-Frenkel model for patchy colloids is extracted from Monte Carlo simulation data. The projections onto rotational invariants of the pair distribution function and the cavity function, $g_{l,l',m}(r)$ and $y_{l,l',m}(r)$, are directly evaluated. The corresponding direct correlation function and bridge function coefficients are obtained by inverting the anisotropic Ornstein-Zernike and closure integral equations. Using this bridge function coefficients, we solved to autoconsistency the integral equations system for the $g_{l,l',m}(r)$, comparing them with simulation results and with the solution of the reference hypernetted-chain approximation based on (optimized?) hard sphere bridge functions.

Shape and orientation of large amphiphilic dendrimers

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Among the many self-organizing supramolecular systems, dendrimers have long been recognized for their ability to condense into a range of crystalline, quasicrystalline, and liquid-crystalline phases. How these phases are formed depends on the details of the internal dendrimer structure and on their effective interactions on the pair level as well as on many-body levels. Using Monte Carlo simulations, we first analyse the internal structure of isolated and interacting dendrimers of different generations for different interaction parameters. Then we focus on bulk systems of fourth-generation dendrimers, where we study the dependence of the structural and orientational properties on the density. Our results show that these dendrimers have an elongated, anisotropic shape. By analysing the spatial distribution of these dendrimers in the fluid phase, we observe that in the first nearest-neighbour shell the density is more elevated perpendicular to the dendrimer's long axis than parallel to this axis. In the second shell this situation is reversed with the density being higher parallel to the long axis.

Two-dimensional transport of paramagnetic colloids via an AC-induced ratchet

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Magnetic garnet films are characterized by a striped magnetisation which can be adjusted through an external homogeneous magnetic field. An oscillating field drives paramagnetic colloids, which perform Brownian motion in a plane above the film, out of equilibrium and induces a ratchet effect [1, 2]. We investigate the dependence of the arising transport on particle interaction. The Gaussian core model is used to define the interaction potential. The Brownian motion is assumed to be overdamped. As a framework for solving the equation of motion for the time-dependent probability density, we employ the dynamical density functional theory where the microscopic particle interactions enter via a free energy functional [3]. Mean squared displacement, diffusion coefficient and other transport properties are calculated in two dimensions and in a one-dimensional cut perpendicular to the stripes of magnetisation. The first results of simulations including attractive magnetic dipole interactions are shown.

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Water cavitation in carbon nanotubes at negative pressures

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The aim of this work is to investigate heterogeneous nucleation of water vapor inside carbon nanotubes. The simulations were performed with the TIP4P/2005, which has been extensively tested during the last years showing it is the most accurate rigid empirical model developed to date. We have combined this water model with carbon potential from OPLS-AA to model the carbon nanotubes. Unlike the TIP4P/2005, the force-fields to model carbon interactions are still subjected to certain level of uncertainty. We have set up configurations of single-wall carbon nanotubes embedded in water and used these configurations to investigate heterogeneous bubble nucleation. We observe that vapour nucleation happens at the walls of the nanotube, deforming it. For a given nanotube diameter, nucleation is only observed at the outer surface of the nanotube and not in the confined region. The latter observation is most likely related to the pressure imbalance across the curved surface. Additional simulations in an *NVT* ensemble have been performed to investigate cavitation inside the nanotube, by adding water inside the nanotube with the same diameter. Further studies have been performed to study the effect of the nanotube diameter on the nucleation rate. In order to measure the nucleation rate at the given thermodynamic state points (corresponding to unstable/metastable water), we computed several cavitation trajectories. These trajectories were analyzed using the volume of the largest bubble as a local order parameter and the mean first-passage time technique in order to quantify the nucleation rate, bubble critical volume and the nucleation barrier.

Dynamic phases of colloidal monolayers sliding on commensurate substrates

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We report on numerical simulations of a monolayer of charge-stabilized colloids driven over a substrate potential by an external DC force. Using overdamped Langevin dynamics we studied the locked-to-sliding transition for various interparticle interaction strengths as a function of the driving force. A detailed analysis of the dynamical trajectories shows that the sliding dynamics is characterized by varying degrees of correlation leading to strongly collective effects. For weak interactions, the diffusion of individual defects is responsible for the motion of the monolayer. As the interaction strength is increased, there is a continuous transition towards distinct density compression and decompression zones are responsible for the motion of the monolayer. For very strong interactions, a type of stick-slip mechanism emerges, in which the sliding of the monolayer is mediated by the propagation of collective distortion waves. Our predictions can be tested experimentally with 2D arrangements of colloidal particles exposed to periodic light fields.

Coarse-graining strategies for coronene molecules

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Coarse-graining describes the idea of systematically integrating out irrelevant degrees of freedom in order to create an effective Hamiltonian, which allows to investigate larger length- and time scales. In this poster we focus on the coarse-graining of coronene molecules from atomistic detail to mesoscopic molecular detail. So far only a complicated, temperature-independent coarse-grained model for coronene, used for static calculations, exists [1]. A hierarchy of model potentials generating different many-particle aspects of coronene, e.g. crystal stability, aggregation, etc., will be introduced. These models are studied via mesoscopic molecular dynamics simulations. As a basic platform for molecular pair interactions, the Gay-Berne potential with electric multipoles, which has been established [2], is used. This ansatz is combined with parameters characterizing the electronic contributions as well as shape contributions from atomistic, biased umbrella sampling simulations. The fitting procedure of the models will be discussed.

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Long-time dynamics and dynamic scaling in suspensions of charged and neutral colloidal particles

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We investigate the time-dependent intermediate and self-intermediate dynamic scattering functions (DSFs), describing the spatio-temporal pair correlations of charged (CS) and neutral hard spheres (HS) both theoretically and experimentally. Extensive Brownian dynamics and accelerated Stokesian dynamics simulations and mode-coupling theory calculations of the DSFs have been performed for a large range of correlation times, for HS and for pair potential parameters representing strongly charged silica spheres in a refractive index matching organic solvent. Our theoretical results for CS silica systems are amended by dynamic light scattering (DLS) data. While the temporal decay of the intermediate DSF is clearly diffusive at short times, the physical nature of its long-time decay is still under debate [1-4]. A DLS study of Segrè and Pusey [1] for HS systems suggests that the long-time decay is diffusive for wavenumbers around and above the principal peak position of the static structure factor, with factorized time- and wavenumber dependence of the relaxation rate. This factorization feature, referred to as dynamic scaling, has been questioned for HS in Refs. [2] and [3], for different reasons. As an approximate feature, it has been observed also for CS suspensions in [4]. To identify the true long-

time decay of the DSFs from experimental and theoretical data is a challenging task [3]. Our comprehensive theoretical-experimental study adds to the understanding of the DSFs and dynamic scaling at intermediate to long times.

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Structure, dynamics and rheology of colloidal dumbbell suspensions

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We investigate the static and dynamic equilibrium structures of a suspensions of colloidal dumbbells by means of Brownian dynamics computer simulations and linear response theory. These suspension exhibit an elaborate equilibrium phase diagram [1, 2]. Recent advances in synthesis and experimental realisation of highly monodisperse adjustable dumbbell suspensions allow access to a wide area of the parameter space [3]. This gives rise to interesting questions concerning structure, dynamics and macroscopic properties. The particular focus is the study of bulk translational and orientational structure and near-equilibrium transport coefficients at different colloid packing fractions and anisotropy parameters for a better understanding of material properties in and out of equilibrium. Crystal structures in the plastic crystal (PC) phase are identified and the PC-liquid transition is investigated. We present structural properties in form of static and dynamic structure factors $S(q, \omega)$ and pair distribution functions $g(r)$. Furthermore we calculate frequency-dependent rotational and translational self-diffusion constants as well as shear viscosities from equilibrium autocorrelation functions. In addition we will present preliminary results of non-equilibrium simulations imposing oscillatory and steady simple shear flow. All results are compared to the hard sphere reference system as well as available experimental scattering and rheology data.

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Hierarchically structured, double inverse composite opals

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Hierarchically structured materials prepared from colloidal particles as building blocks or templating objects are currently investigated for a vast range of potential applications. In this direction, we have been studying various strategies to prepare colloidal hierarchies, and present here a versatile and simple method to fabricate porous composite materials with a hierarchical ordering on several length scales. The fundamental templating motifs are colloidal assembly structures, which can be conveniently accessed by well-established convective assembly methods. We demonstrate the preparation of inverse opal structures with a range of materials, such as SiO₂, TiO₂, and Al₂O₃. Furthermore, this host matrix can be further infiltrated and modified by a second type and size of particles, yielding a drastically finer structured, intercalated phase with a superlattice. Yet, this second phase can serve as a template to be replicated into a sophisticated porous material. These sequential infiltration and removal steps allow for a vast combination of inorganic solid phases. Their multi-level structuring at several length scales holds promise for applications in catalysis or photovoltaics, where hierarchically structured interfaces play a crucial role. Finally, the complex hierarchical material can be inverted to its polymer replica by monomer infiltration and polymerization.

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Self-assembly scenarios of patchy colloidal particles

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The rapid progress in precisely designing the surface decoration of patchy colloidal particles offers a new, yet inexperienced freedom to create building entities for larger, more complex structures in soft matter systems. However, it is extremely difficult to predict the large variety of ordered equilibrium structures that these particles are able to undergo under the variation of external parameters, such as temperature or pressure. Here we show that by a novel combination of two theoretical tools, it is indeed possible to predict the self-assembly scenarios of patchy colloidal particles: On one hand, a reliable and efficient optimization tool based on ideas of evolutionary algorithms helps to identify the ordered equilibrium structures to be expected at vanishing temperature; on the other hand, suitable simulation techniques allow to estimate via free energy calculations the phase diagram at finite temperature. With these powerful approaches we are able to identify the broad variety of emerging self-assembly scenarios for spherical colloids decorated by four patches and we investigate and discuss the stability of the emerging crystal structures on modifying in a controlled way the tetrahedral arrangement of the patches.

On the temperature maximum of magnetic susceptibility in dilute systems of dipolar hard spheres at low temperature

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We employ the combination of density functional theory and Monte Carlo simulations to elucidate possible structural crossovers for systems of dipolar hard spheres and the influence of these crossovers on the temperature dependence of the initial magnetic susceptibility. We found that at low densities, when the temperature starts decreasing, the initial susceptibility grows due to the enhanced chain formation. However, when the temperature drops sufficiently, rings start forming. Every ring has a zero dipole moment and, as that, has almost zero initial susceptibility. The redistribution of particles from chains to rings can be interpreted as the appearance of magnetically inert particles (those in rings). Thus, the overall decrease of the volume fraction of magnetically “active dipoles” leads to the decrease of the initial susceptibility. We investigate thoroughly the region of the susceptibility maximum for various densities, and put forward the concept of “magnetically inert” particles also for higher densities, those that form clusters with on average zero total dipole moment. At higher densities, though, instead of rings, complex branched networks were observed in the simulations. This study allowed us to explain various experimental evidences of the nonmonotonic temperature behaviour of magnetic susceptibility in ferrofluids.

Hydrodynamic synchronization of non-spherical colloids

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During the past decades, many physical experiments in colloidal science have been done with laser optical tweezers and colloids containing hard-walled spherical particles. However, trapping of non-spherical particles is both very different and much less mastered than that of spheres. Physicists, biologists, engineers and other scientists are interested in trapping of elongated particles because it can serve as a model system for the study of fundamental hydrodynamic phenomena in biological samples, furthermore due to propagating applications of nanotubes and nanorods in biophysics, microfluidics, photonics and microelectronics. The primary purpose of the study was to examine the synchronization of hard-walled non-spherical dielectric (ellipsoid-like) particles, of few tens of micrometers in length, trapped by a laser beam and to find an analogy with the motion of artificial cilia. Acousto-optic deflector offers the possibility to have more traps, i.e. to have more “active” particles in the experiment. Experiments with different number of particles were executed. By one-particle experiment the goal was to demonstrate the correlation between certain physical values such as frequency, amplitude and laser power. Furthermore, by two-particle experiments we demonstrated the strength of synchronization for different positions (left-right, up-down, diagonal) and for various mutual distances between particles. The synchronization was observed for few (2, 3) and several (up to 20) particles in a variety of configurations – an array of particles, circular/ellipsoidal matrixes – for different mutual distances, particle orientations, and no external input.

Simulation of C₆₀ non-equilibrium surface growth

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Kinetic Monte Carlo simulation methods allow the simulation of non-equilibrium epitaxial surface growth over experimentally realized time spans of minutes and growth of multiple layers of particles [1]. Through variation of simulated temperature and adsorption rate the structures formed can be manipulated and predictions for experimental methods such as molecular beam epitaxy can be made. We apply the method to simulate multilayer growth of C₆₀. The material parameters are obtained through comparison with grazing-incidence X-ray scattering measurements [2]. The simulations allow for a time-resolved analysis of the real and reciprocal surface, geometric and statistical analysis as well as an understanding of microscopic processes obtained from particle trajectories. Characteristic time-dependent features such as the average island distance and layer filling fraction are consistent with the experimental data for long time spans and several temperatures.

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Aggregation of rigid block copolymer stars

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Diblock copolymer stars in solution – with a solvophilic A block and a solvophobic B block – show a manifold phase behavior, reaching from macrophase separation and micellization to percolating macrogel structures. The physical parameters allowing tuning of the single-molecule properties as well as those of concentrated solutions of the same are the arm number, the fraction of attractive end-monomers and the rigidity of the arms. We present computer simulations of single molecules as well as in the grand canonical ensemble. By tuning the number of arms and the size ratio of the A and B blocks, we calculate phase diagrams and examine the influence of the stars' arms' bending rigidity on phase behavior and morphology. We find that for macrophase separating systems an increase of the rigidity leads to a rise in the critical temperature as well as a lower critical density. We also find systems with no critical effects in the full flexible case that show critical behavior when applying bending rigidity, as well as systems that feature multiple critical points when becoming very stiff. Furthermore we conduct morphological studies of micellar mixtures and examine the influence of the rigidity on the micelles' ability to inter-aggregate.

Equilibrium planes and microchannels in inverse patchy colloid systems

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Heterogeneously charged entities, such as micelles, vesicles, colloids and globular proteins in solutions, are ubiquitous in nature and the understanding of their collective properties is essential for many technological and natural processes. Here we consider colloidal particles with a negatively charged equatorial region and two positive polar caps; we refer to them as "inverse patchy colloids" [1] since regions with like charges repel each other while oppositely charged regions attract each other. We model the system via a recently introduced coarse-grained description [1] and we investigate the effect of the interplay of directional attractive and repulsive interactions on the equilibrium phase diagram. Via a novel combination of evolutionary algorithms and Monte Carlo simulations [2], we are able to identify regions of thermodynamic stability for a variety of structures, among which planar structures and dense phases with percolating parallel channels seem most striking with respect to immediate technological applications. Using a suitable thermodynamic integration scheme [3], we have calculated for selected system parameters phase coexistence between competing ordered and disordered structures.

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Theoretical analysis of the facets of the cubosomes

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Shapes of the cubosomes, dispersed particles of cubic liquid crystalline phase, can be investigated theoretically. Using a program developed in our group we performed a theoretical analysis of the facets in directions [111], [110], and [100] for different cubic phases, in particular for phases P and D. It was also shown how the structure of the cubic phases is modified by the presence of facets. Calculations for different sizes, different orientations, and different boundary conditions for droplets of cubic phases surrounded by water where the shape of the droplet was modeled by different polyhedral which were observed in experimental studies were performed as well as calculation of the genus, surface area, Gaussian and mean curvatures for these structures.

New lattices in colloidal artificial spin ice

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We study new lattices in the colloidal version of artificial spin ice. These lattices exhibit interesting ground states and excitations, and contain a built-in frustration of geometric nature. Due to this frustration, defects appear on the lattice as all constraints cannot be simultaneously satisfied. This creates possibilities of interesting manifold ground states and creates excitations that are always present on the lattice. We calculate the residual entropy of these systems and show the ground states, the location of the excitations in the ground states and their possible dynamics for small perturbations (small temperatures and fields). We show that by designing the lattice geometry, new types of frustrated ground states can be created which are interesting for the broader field of spin ice physics.

Measurement of the four-point susceptibility of an out-of-equilibrium colloidal solution of nanoparticles using time-resolved light scattering

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Characterizing the complex behavior of soft condensed matter requires the development of refined conceptual and experimental tools. Many systems of wide theoretical and practical interest like supercooled liquids, colloids, polymers, etc. exhibit complicated structural and dynamical features. In particular, the motion of the constituting elements of these systems (atoms, macromolecules, monomers, etc.) might be characterized by large spatial heterogeneities displaying large fluctuations in space. This implies that in some regions of the system the dynamics proceeds very slowly, while elsewhere it can be notably faster. The experimental investigation of these features turns out to be very challenging, and few studies have established evidence of dynamical fluctuations significantly larger than the molecules' size. On the other hand, computer simulations have investigated intensively the heterogeneous scenario described above. Multipoint correlation functions and, in particular, the four-point susceptibility have been used to characterize the spatially heterogeneous dynamics in computer simulations. Here we present an experiment capable of measuring directly the four-point susceptibility in off-equilibrium nanoparticle colloidal suspensions [1]. In this case, the approximation schemes [2] for the four-point susceptibility recently proposed, based on equilibrium properties, are not applicable since the system is aging. We measure directly the four-point susceptibility without resolving the positions of the individual particles. The experiment employs two

different dynamic light-scattering techniques by combining heterodyne and homodyne photon-correlation spectroscopy. The idea of the experiment is to use a very small scattering volume in order to enhance the sensitivity in measuring dynamical fluctuations: The smaller the studied volume, the larger are the non-Gaussian components of the fluctuations. The experiment is performed on an ageing low-concentration colloidal solution of laponite, which is a synthetic clay that has been studied intensively for its rich dynamical and structural behavior as well as numerous applications.

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Structural and dynamical properties of polymer-colloid nanocomposites

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We investigate the equilibrium and rheological behavior of polymer/colloid nanocomposites. In particular, we focus on a mixture of multiarm star polymers mixed with smaller spherical colloidal particles, thereby reverting the usual scenario in which the polymers act as depletants to the colloids [1]: Here, the hard colloids act as small additives to the big stars. We develop a coarse-graining model to describe the effective interactions of hard colloidal particles next to polymer stars, dependent on two main parameters: The size ratio q between colloidal particles and stars and the number of polymeric arms f . Theoretical considerations of the radial dependence of the osmotic pressure inside a star together with monomer-resolved simulations [2] provide us with a full coarse-grained theory of colloid/star interactions for a wide range of the parameters q and f [3]. Combined with the known star-star and colloid-colloid interactions (modeled as hard spheres), the coarse-graining allows us to make predictions about the structure of the binary mixture and in particular about the influence of hard additives on the structure and rheology of soft polymers with the help of the Rogers-Young integral equation and coarse-grained simulations. By combining our structural data with mode coupling theory, we investigate the effect of the added colloids in modifying the glassy behavior of the polymer matrix.

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Wetting dynamics of ellipsoidal polystyrene particles

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The partial wetting configuration of a solid particle across an interface (water-air, typically), is a standard problem in the physics of capillarity. As well known, the geometry of the particle-interface system is of paramount importance as the source of capillary interactions between particles located at interfaces and in determining the lifetimes of particle-stabilized films and emulsions. The emersion time of an ideal sphere of radius a is expectably of the order of $\eta a/\gamma$, where η is the fluid (water, say) viscosity and γ the interfacial tension. However, recent experiments by Kaz et al. [1] with micrometer-sized spherical particles have revealed that the process is much slower, due to small heterogeneities of particle surfaces, leading to transient contact line pinning. Independently of surface defects, spheres are a very special case, due to their symmetry and the fact that emersion may proceed through a continuous series of planar (circular) contact lines. Most of real particles are non spherical: This makes emersion more complex, as it involves up to 4 degrees of freedom for the particle itself, and because partial wetting of the particle body is not compatible with planar contact lines [2, 3]. In this communication, we report observations with polystyrene particles, which are initially suspended in bulk water and individually manipulated by a laser beam, using laser radiation pressure [4]. The experiment amounts to picking up a particle and make it rise up to contact to the water-air, or water-oil, interface. We then observe the dynamics of particle breaching through the interface, until stabilization. Events are recorded as microscope video images of the particle, in transmission or reflection modes, complemented by interferometric maps of the interface distortions. Fast steps, beyond

highest available video rate, are recorded from the variation of the transmitted laser beam intensity through a pinhole. We report data obtained with spheres ($a = 5 \text{ }\mu\text{m}$) and with ellipsoids of increasing aspect ratios (up to $30 \text{ }\mu\text{m}$ in length). The dynamics of sphere emersion is found in line with former observations [1], featuring a logarithmic increase of the dry area dimension. We observed that the emersion of ellipsoids would depend on their dynamics below the interface [4], indicating that breaching depends on the way in which the particle initially gets in contact with the interface, as put forward in Ref. [5]. In general, breaching starts with the particle at an angle with the interface and proceeds through increasing of the contact line. Ultimately the particle gets aligned parallel to the interface. However, transient large protrusion of the particle in air, predicted in simulations [5], is not observed.

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Complex industrial colloidal systems in intense centrifugational fields

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A huge variety of products containing submicrometer particles are nowadays produced in industrial processes all around the world. Such colloidal particles are typically used in products to help bind, stabilize, coagulate, suspend, thicken, and form films. The physical properties of such nanoparticles can therefore to a large extent define the end property of the product. Here we demonstrate that investigating complex colloidal systems by means of analytical ultracentrifugation can deliver valuable information not accessible by common techniques.

Energy landscapes, structural topologies and rearrangement mechanisms in clusters of dipolar particles

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Clusters of spherical particles with isotropic attraction favour compact structures that maximise the number of energetically optimal neighbour interactions. In contrast, dipolar interactions lead to the formation of chains and a low coordination number. When both isotropic and dipolar interactions are present, the competition between them can lead to intricate coil, knot and link structures. Here we investigate the evolution of the energy landscape of clusters bound by the Stockmayer potential (Lennard-Jones plus point dipole) as the strength of the dipolar interactions is changed, using disconnectivity graphs to visualise the organisation of the landscapes. From comprehensive surveys of isomerisation pathways, a number of rearrangement mechanisms can be identified that allow the topology of chain-like motifs in the structures to be modified, giving insight into how topologically complex structures might self-assemble.

Macroscopic properties for magnetic fluids: Pressure and initial magnetic susceptibility

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Ferrofluids are colloidal suspensions of magnetic nanoparticles (typical size 10-20 nm), usually stabilized by steric coatings (in non-electrolyte carrier liquids) or by electrical double layers (in aqueous solutions). Capability of ferrofluids to hold liquid properties under influence of magnetic fields is a base of its applications ranging from engineering to biomedicine. This denotes a reason of an intense interest for theoretical and experimental investigation of its properties. Real ferrofluids are polydisperse, but influence of polydispersity can be observed even in bidisperse systems composed by magnetic particles of two different sizes [1]. Earlier works demonstrated that the behavior of monodisperse ferrofluids could differ sufficiently from the one of bidisperse systems: As an example, more active chaining in monodisperse systems, differences in ground states of these systems [1-3]. Another important factor which influences the cluster formation is the geometry of the sample: In a bulk or in a monolayer (a thin layer). In Ref. [2] it was shown that the crossover from a bulk to a monolayer leads to changing of the aggregation mechanism. Specifically, in bulk the main part in this process plays the energy, whereas in a monolayer the formation of aggregates is predominantly driven by entropic factor. In the present study we elucidate how polydispersity and geometry of samples influence the experimentally measurable macroscopic properties such as pressure and initial magnetic susceptibility of the magnetic dipolar particle system. To perform that, we employ molecular dynamics computer simulations,

using the simulation package ESPResSo [4], in combination with theoretical calculations of these properties. We consider a wide range of particle concentrations and dipolar strength. This makes it essential to use two different approaches for the theoretical pressure and susceptibility calculations: The method of diagram expansion of the magnetic dipole-dipole interaction for small concentrations and low dipolar strength and, the classical density functional theory for large ones. Comparison of the obtained theoretical results and simulation data leads us to deeper understanding of the pressure and susceptibility dependencies on the aggregate formation, system polydispersity and geometry of samples.

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Stabilisation of ordered colloidal structures and deformed defects by polymerisation of reactive liquid crystalline matrices

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Colloidal assemblies in anisotropic media are kept together by a balance between repulsive electrostatic interaction and attractive van der Waals forces. In nematic liquid crystalline matrices colloidal particles can be assembled exploiting the elastic distortion of the nematic director. By means of laser tweezers is possible to guide the assembly process allowing a one-by-one formation of 2D colloidal crystals [1]. However, these assemblies are only stable in the media they are assembled. We present a new method for the stabilisation of such assemblies based on the polymerisation of the liquid crystalline matrix. Mono- and difunctionalised liquid crystalline monomers were dispersed in a nematic liquid crystal (5CB). Silica particles functionalised with a photoinitiator were dispersed in the reactive mixture and assembled using laser tweezers. Irradiation of the cell with UV light yielded an aligned polymeric network which embedded the assemblies and preserved their patterned structure as demonstrated by diffraction of light. The network has been also proven to be thermally stable. Partial polymerisation of the matrix has also been used to stabilise the deformation of topological defects. The irradiation of the cell for a limited period of time increases the viscosity in particular near the surface that was irradiated allowing the formation of a polymeric layer. Using laser tweezers is possible to pull the topological defect present around a particle and at the same time create a preferential pattern on the polymeric layer where the defect pins, the defect

maintained a certain degree of elasticity and when released tended to return to its original position. Further irradiation of the matrix while the defect is pulled induced the complete polymerisation of the matrix stabilising the defect in unconventional fashion.

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Field-induced assembly of magnetic colloids

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Controlling colloidal interactions is one of the main challenges in colloidal science. Traditionally interactions among colloids are tuned via ionic strength, pH, adding polymers and similar. A different approach would be to use the external electric or magnetic field. Osterman et al. experimentally investigated the self-assembly of superparamagnetic colloids in precessing magnetic fields [1]. We are trying to explain their results from theoretical point of view through numerical simulations. We performed Langevin dynamics simulations on two- and three-dimensional systems of superparamagnetic hard spheres in precessing magnetic field. We investigated structures formed in two-dimensional systems at different opening angles of precessing field. In accordance with the experiment we observed the repulsion, formation of single chains, branching of chains and formation of percolating networks when going from 0 to 90 degrees of opening angle. Another interesting experimental observation was the formation of rotating symmetrical clusters (hexagons) in the precessing magnetic field [2]. In contrast to the asymmetric clusters it is not immediately obvious why would symmetric clusters rotate in the precessing magnetic field. Tierno et al. presented a theoretical explanation for rotating symmetric clusters [2]. To see whether their theory is valid we decided to perform numerical simulations of their model and test theoretical predictions.

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Colloidal particles in near critical solvents

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We consider colloidal particles immersed in a binary liquid mixture which exhibits a miscibility gap. Close to the critical point of demixing, the solvent exhibits long-range correlations. The critical fluctuations spectrum and the profile of the order parameter of the binary liquid mixture is affected by the presence of the colloidal particles. By making use of different methods, it is shown that such colloidal suspensions exhibit a fluid-fluid phase transition into a colloidal rich and a colloidal poor phase. Further, it is shown that the corresponding order parameter is a combination of the concentration of the solvent particles and the density of the solute particles.

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Ordered cluster forming systems under external pressure

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The formation of stable clusters by ultrasoft particles has received much attention during recent years [1]. The existence of ordered and disordered arrangements of clusters formed by partly or fully overlapping particles in the absence of attractive forces seems counterintuitive at first sight, but is meanwhile fully understood. One of the most intriguing features of ordered cluster phases is the density independence of the lattice constant: Upon compression the lattice constant remains constant while concomitantly the cluster population increases [2]. To be more specific, under pressure clusters dissolve and the liberated particles join other clusters. So far, this prediction has only been verified in *NVT* simulations. In this contribution we study the effect of an external, variable pressure on different types of cluster forming particles. In our investigations we have focused on amphiphilic polymers, which have been treated both on a monomer-resolved as well as on a coarse-grained level. The pressure and the temperature are tuned via a combined thermo-barostat, formed by ideal gas particles which interact with the ultrasoft colloids via an inverse power law [3]. Starting at low pressure (and a correspondingly low density) we compress the system until it passes the fluid/cluster-BCC transition line. Upon compression the system undergoes a cluster-BCC to cluster-FCC transition. An even further increase of the pressure makes clusters melt, liberating thereby individual particles, which, in turn, join neighbouring clusters and increase thereby their occupancy. The use of molecular dynamics simulations allows to investigate this process in detail and to trace the trajectories of the individual particles.

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Temperature controlled colloidal deposits by weak AC electric fields

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Charged colloidal particles are sensitive to external electric fields even at higher temperatures. The effect of a weak AC electric field on a diluted dispersion at low temperatures (20-40 °C) with a free surface leads to the formation of clusters along the contact line [1], where the life time of clusters depends on the allow temperature. We obtain the dried structure of dilute colloidal suspension through evaporation at higher temperatures (50-60 °C) by weak AC electric field controlling the motion of particles for deposition. As a result, long columns of particles are deposited on the substrate. Experiments show that at higher concentration (1.1%) and temperature (60 °C) due to rapid evaporation rate particles through capillary action packed close enough to form well dried depositions. On the other hand at moderate concentration (0.5%) and temperature (50 °C), there is trapping of thin film of liquid inside the deposition. We report experimental results on characteristic length between these clusters and columns, which are changing as the concentration and applied field change. We are interested to demonstrate the flow of particles during deposition as a function of temperature [2].

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Ground state structures of the three-dimensional Stockmayer fluid

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Self-assembly is the fundamental principle which generates structural organization on all scales from molecules to galaxies. It is defined as reversible processes in which preexisting parts or disordered components of a preexisting system form structures of patterns. The self-assembled systems composed by magnetic nanoparticles are particularly interesting and have been used as a potential applications in magnetic fluids, data storage and for a number of biological and medical applications. The striking feature of magnetic nanoparticles is that their interaction can be both repulsive and attractive, depending on the respective orientation of the magnetic moments of particles. Another important advantage is that their interaction can be tuned by an external magnetic field which orients the particles and therefore controls the physical properties of the system. These characteristics provide a set of tools to design and synthesize new assembled structures with desired shapes and components. We study the ordered configuration of magnetic particles in three dimensions as function of the magnetic moment of the particles. The structure of clusters is analyzed in systems with different number of particles. We find very non-trivial configurations like parallel rings and catenanes. Independently of the number of particles, the perpendicular rings occur in a range of the magnetic moment values. We show that the system presents ring configuration even for small number of particles. Besides, the growing of the number of particles with low magnetic moment

indicates to follow a pattern which the symmetry of structure plays an important role. Similar structures are summarized in a phase diagram which indicates that the chain configuration is may be presented by systems with any number of particles. We show that the system presents structural transitions before particles align completely with the magnetic field when its intensity is increased. Besides inducing a line-shaped structure, we find that the magnetic field may organize the system in parallel rings organized in the perpendicular direction of the field. A phase diagram summarized the structures of systems with different values of magnetic field and number of particles. This diagram indicates that the chain configuration in large clusters is obtained with large values of the magnetic field after presenting ring structure.

Mobility and diffusion coefficients in three-dimensional magnetic fluids

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The investigation of the diffusion in magnetic fluids is crucial for medical applications. There were several attempts to study diffusion [1-5], but the detailed theoretical description is still missing. We study the mobility and diffusion in the three-dimensional magnetic fluids with chain aggregates, both for model mono- and bidisperse systems, using the density functional approach. Firstly, we calculate mobility coefficients in the mono- and bidisperse systems, employing the formulas which were analytically derived by Perrin [6]. We find that in the monodisperse system the mobility decreases with increasing particle volume fraction, and it increases in the bidisperse magnetic fluid. It means that even on the level of self-diffusion, the system polydispersity exerts an influence on the particle and aggregate mobility. This behavior of the mobility is related to the fact that the average chain length in the monodisperse system increases with the volume fraction, whereas, for bidisperse ferrofluids, it might significantly decrease, depending on the granulometric composition. Secondly, we investigate in detail gradient diffusion, using the mobility coefficients obtained in the first part. We show that depending on the gradient-type and polydispersity, diffusion coefficients could exhibit qualitatively different dependence on the ferroparticle density. Finally, we exploit obtained diffusion coefficients to describe possible distribution of aggregates in the gravitational field. We perform an extensive comparison of our theory and results of molecular dynamics and Monte Carlo simulations. The research was supported by the

Ministry of Education and Science of Russian Federation (Project No. 2.609.2011), RFBR Grants (No. 12-02-31374 and No. 12-02-33106), and FP7-IDEAS-ERC Grant PATCHYCOLLOIDS.

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Ring polymers in solvents of varying quality

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We employ extensive computer simulations to investigate the conformations and the interactions of ring polymers under conditions of worsening solvent quality, in comparison with those for linear polymers. We determine the dependence of the theta temperature on topology by considering ring polymers of different topologies. We establish a clear decrease of the same upon changing the topology of the polymer from linear to an unknotted ring but a very weak dependence on modifying the knottedness to increasingly complex knots. Our results are based on two independent methods, one by considering the scaling of the gyration radius with molecular weight, and one based on the dependence of the effective interaction on solvent quality. In addition, we calculate several shape parameters of the polymers to characterize linear, unknotted and knotted topologies in good solvents and in the proximity of the theta point. The shape parameters of the knotted molecules show an interesting crossover at a degree of polymerization that depends on the degree of knottedness of the molecule.

Percolation thresholds and critical exponents of colloidal suspensions in bulk and confinement

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We performed extensive grand canonical Monte Carlo simulations to investigate the percolation transition of spherical colloids (i) in the bulk phase and (ii) confined between two parallel, structureless walls (slit pore) [1]. The interaction between the colloids is modeled through a square-well potential with an attraction range of only 4% of the hard core diameter to mimic the ultra-short ranged nature of depletion attractions, which are of great importance to colloid-polymer mixtures [2]. Applying a finite-size analysis, we investigated the density threshold of the connectedness percolation at several width of the slit pore at fixed temperature. Increasing the wall separation, we found a shift of the percolation threshold towards the bulk value obtained from an unconfined, in other respects identical system. We could explain this shift by scaling arguments, which are usually applied in the framework of cross-over scaling of the vapor-liquid critical point of simple liquids in slit pores [3]. We also studied the critical exponents of the percolation transition and found them to be notably insensitive to the width of the slit pore.

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Structure and equation of state of hard disks under adaptive confinement

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By combining real-space experiments and Monte Carlo simulations, we present a two-dimensional colloidal system confined by a soft circular boundary. This boundary is defined using holographic optical tweezers, resulting in a deformable elastic wall. Such adaptive confinement has important consequences. Its elasticity leads to a bistable state, and we directly obtain the radial osmotic pressure of the confined fluid. We further find a first order phase transition between a hexagonal structure reminiscent of the bulk and a concentrically layered fluid mimicking the shape of the confinement.

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Density-dependent interaction between colloidal particles on an oil-water interface

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The study of physical properties of interfacially trapped micro and nanoparticles at liquid-liquid interfaces has received significant attention in recent years for their possible applicability to industrial and technological problems as well as to their use as (quasi-)two-dimensional model systems for investigating questions of relevance in condensed matter physics. The understanding of the interactions that determine the stability behaviour of colloidal particles at water/oil interfaces is highly desirable and remains surprisingly poor for a relatively simple physical chemistry system. We investigate a system made of PS colloidal particles at the decane-water interface; the radial distribution function, $g(r)$, is measured by optical microscopy, and the pair interaction potential is obtained from the inversion of this input structural data. This ensemble method differs from another common approach, which can be found in the literature, where a direct measurement of the pair interaction is performed using optical tweezers: The forces acting between two particles are obtained directly, in this case, but neglecting possible many-body effects that occur at finite particle concentration. By measuring the pair correlation function $g(r)$ for different densities of PS particles at the decane-water interface, and using a powerful predictor-corrector inversion scheme, we show that the effective pair-interaction potential is strongly density dependent as soon as the system is not dilute. A long-range minimum develops reaching a depth of several $k_B T$. The complexity of the

interaction potential, which had been previously assumed to be a simple dipole-dipole interaction, is confirmed by quantifying the mobility of colloids confined by their neighbours and by the presence of sharp interfaces between regions dense in colloids and macroscopic areas devoid of particles. We discuss the possible origin of this effective attraction as a many-body effect linked to interface deformation.

Dynamics of Pac-Man lock-and-key colloids: The role of the solvent

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Translational and rotational dynamics of a two-dimensional model of Pac-Man lock-and-key colloids [1] have been studied via molecular dynamics and fluid particle dynamics [2] simulations. Formation of chains and difficulty of aggregation can be traced back to the effects hydrodynamic interactions controlled by the solvent viscosity.

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Prediction of nanofiber production based on interfacial rheological measurements

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Nanofibers are solid fibers with nanometre-scale diameters, theoretically unlimited length, large surface area-to-volume ratio and high porosity. Due to their physical characteristics, nanofibers can be used in the chemical, textile, computing, biomedical and pharmaceutical industries [1, 2]. The method, most commonly used for nanofiber preparation is electrospinning, which produces nanofibers from polymer solutions due to connection with a high-voltage supply. Applied voltage results in prevalence of repulsion forces in polymer solution over the forces, maintaining the spherical shape of a droplet. Firstly a Taylor cone is formed, then a continuous jet of polymer solution, which is accelerated towards the grounded collector [1]. The success of the electrospinning process (smooth, beadless nanofibers) depends on many different but interrelated parameters of solution, process and environment, therefore prediction of electrospinning product is very complex and difficult. In our research interfacial rheological characteristics of polymer solutions were investigated and correlated with nanofiber morphology to evaluate their prediction power. Interfacial rheological characteristics of polymer solutions (interfacial η , G' and G'') seem more important than classical bulk rheological characteristics, since a significant increase in the surface-to-volume ratio occurs during jet formation in electrospinning process ($S/V = 4D-1$; S – jet surface, V – jet volume, D – jet diameter). The jet diameter is reduced from approximately 1 mm (inner diameter of the needle used) to a few hundred nanometres or less (diameter of produced nanofibers). Moreover, solvent evaporation causes a concentration gradient of polymer molecules in the electrospun jet,

which is exerted in its interfacial characteristics. We have found out that interfacial η detect changes in polymer solution with greater sensitivity than classical η and that for successful electrospinning, the polymer solution should show greater plastic properties over elastic (interfacial $G'' \gg$ interfacial G'). Based on investigation of chitosan/poly(ethylene oxide) blended polymer solutions we have proven that interfacial rheological parameters correlate much better with the product of electrospinning process than classical rheological parameters, therefore, interfacial rheology of polymer solutions is a suitable tool to be used for prediction of electrospinning and nanofiber quality.

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Complex nematic structures induced by Laguerre-Gaussian optical tweezers

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Complex optical beams can produce highly nonuniform electric field profiles on micrometer and submicrometer scale that can be used for the formation of complex nematic structures [1]. We demonstrate the formation of various complex nematic structures using Laguerre-Gaussian beams. The optical beam polarization winding number directly imprint into the profile of the nematic director, producing complex symmetric arrangements of nematic defect loops inside optical beam which number is exactly equal to polarization winding number [2]. The role of the optical beam absorption is also addressed, demonstrating complex local heating and “softening” of the nematic within the optical beams. Generally by increasing either beam intensity or absorption in nematic, the region of an effective coupling between the nematic and optical electric field increases. Furthermore, this imprinted director fields turns out to be great initial condition for new complex nematic structures stabilised by colloids and/or chirality. To conclude, using modelling to find stable defect structures based on the delicate balance of the effects due to chirality, confinement, surface anchoring profiles, external fields, and presence of colloidal particles may lead to use in various fields of photonics, optics, and complex material design.

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Dynamics, structure, and rheology of an ageing colloidal glass

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It is well known that in a variety of liquids, the structural relaxation slows down dramatically upon reducing temperature or increasing concentration, while beyond the liquid-glass transition crystallization is suppressed by an intervening glassy state. The latter is often ageing as evidenced by intrinsic dynamics slowing down with waiting time after some appropriate “rejuvenation”. Here, we study the evolution of intrinsic dynamics and structure of an ageing colloidal soft-sphere glass. Asymmetric amphiphilic PEP-PEO diblock copolymers form kinetically frozen micelles in water with a very small core-to-corona ratio [1]. The micelles can be considered as stable colloidal entities and interact via a potential which is identical to regular multi-arm star polymers. At high number densities, the star-like micelles form colloidal glasses as evidenced by rheology and dynamic light scattering measurements. These glasses can be rejuvenated, i.e. brought to a reproducible initial state by thermal treatment. We measured the evolution of the structural relaxation of ageing star-like micelle glasses by multi-speckle dynamic light scattering (MSDLS). The advantage of MSDLS over regular dynamic light scattering is that a correct ensemble-averaged correlation function can be obtained even when the dynamics of the sample are frozen. As expected, after rejuvenation the structural relaxation time was found to increase with waiting time. However, we show that for waiting times longer than a few days (depending on the volume fraction) the relaxation time reaches a plateau and then starts to decrease. The dynamics of the glass continue to speed-up even up to

a month after rejuvenation. This has also recently been observed in regular multi-arm star polymers [2]. Small-angle neutron scattering and rheology experiments were performed to follow the evolution of structure and mechanical properties of the same ageing colloidal glass under similar conditions.

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Flow induced structure formation in low density colloidal suspensions

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Flow induced structures in colloidal suspensions are of significant technological interest as they are ubiquitous in daily life including food, cosmetics, clays, emulsions, paints, surfactant aggregates and medicines, and also represents an important challenge in non-equilibrium statistical physics. We study colloidal suspensions at low densities in the presence of simple shear, using Brownian dynamics simulations. The colloids are modeled as hard spheres interacting through a modified Stillinger and Weber (SW) potential [1]. At low shear rates, the particles first arrange as lanes of beads along flow direction and coarsens along vorticity direction to form bundles. At higher shear rates, bands appear perpendicular to the vorticity direction. When the SW potential is replaced by soft interactions which has short range attraction and long range repulsion [2], at low density limit, with the presence of shear they exhibit lamellar or columnar structure, but now the layers perpendicular to the velocity gradient direction.

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Predicting crystals of Janus colloids

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A successful bottom-up strategy for colloidal molecules [1] requires two main steps: (i) the synthesis of the colloidal molecule and (ii) the prediction of the phase behaviour of the designed particles. As a contribution in the direction of solving step (ii) we present the first thorough investigation of the phase behaviour of patchy colloids, including ordered, partially ordered and disordered phases. Specifically, we focus on hard spherical Janus colloids with one attractive hemisphere. The low-density self-assembly of these particles has been investigated in the past [2-3] and the formation of micelles causing gas-liquid phase separation with a re-entrant behaviour has been observed. We now implement a wealth of different techniques to predict the possible crystal structures for the same model. Beside educated guesses, we implement the floppy box method [4], which allows us to generate a wide set of possible crystals. We also explore the self-assembly of crystal nuclei from fluid and solid initial states. We perform free energy calculations and thermodynamic integration methods for all crystal structures to design the coexistence curve in the pressure-temperature and temperature-density planes. Despite the simple particle design, we find several different stable crystals, all based on underlying hexagonally-close-packed or face-centred-cubic lattice. These crystals differ in the particle orientation and often require correlation between the particle orientations that extend over more than ten particle diameters. In addition to these crystal phases we find a new, surprising wrinkled bilayer, low density structure, competing with both fluid and close packed crystals. This open structure interfere with the micellar gas-liquid equilibrium, suppressing the expected lower

gas-liquid critical point. We also present novel methodological approaches for evaluating the free energy of the micellar phase [5] and the free energy of the wrinkle bilayer phase [6]. These new methods allow us to estimate the low temperature phase diagram in full details [7].

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How particles shape influences the microstructure and macroproperties of magnetic colloids?

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Anisotropic particles form the cutting edge of dipolar soft matter research as they correspond completely to the idea of fine tuning and designing new materials with controllable properties. In this contribution we present a theoretical study and computer simulations on the microstructure and macroproperties of magnetic ellipsoids and cylinders. As the first step, the analysis of the possible ground state structures (the most energetically favored configurations at 0 K) for two and three dimensions is carried out. It was shown that the ground state structure depends not only on the number of particles (as for the system of magnetic spheres) but also on the particle shape anisotropy. Then, for the room temperature we propose a method of calculating the pair correlation function for the combination of Gay-Berne and magnetic dipole-dipole potential based on the group integral technique. It is for the first time to our knowledge, when the anisotropy of the steric repulsion is handled in this way. Using our previous theoretical model for linear chains from magnetic particles, we investigate magnetization and initial susceptibility. To verify our theoretical predictions we perform molecular dynamics computer simulations for dipolar Gay-Berne particles in ESPResSo and extensively compare obtained results. If the dipole-dipole interaction is strong, various aggregates might form both in the systems of shape-anisotropic particles. We are currently actively working on the density-functional theory approach to elucidate the cluster distribution, their topology and

their influence on the macroscopic responses of the system. We prove that even slight shape anisotropy can lead to the drastic change in the microstructure and, as a result in macroscopic responses of the system. Depending on the asphericity of particles and their density both the ground states and the equilibrium room temperature properties can be changed and effectively controlled.

Computing Gibbs free energy differences between phases by interface pinning

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We use a novel approach for computing the Gibbs free energy difference between phases of a material. The idea is to compute the force acting on an interface separating two phases of interest. This force is proportional to the Gibbs free energy difference between the phases and is determined by applying an external field biasing two-phase configurations. The method is validated for the Lennard-Jones model, and we demonstrate the accuracy, efficiency and practical applicability of this approach by computing phase diagrams of a coarse-grained model of DNA functionalized nanoparticles.

Depletion interaction and polymer chain flexibility

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Non-adsorbing neutral polymers such as polyethylene glycols or polysaccharides such as dextrans are used to precipitate colloidal particles including proteins from a suspension. Neutral polymers are depleted from the region between two colloidal particles due to their size, and this depletion in turn exerts an osmotic force capable of bringing colloids together. Several studies has been conducted to address this phenomenon, ranging from theoretical [1-3] to experimental ones [4]. Various aspects including polymer length and composition of the suspension were taken into account. In this work an effect of polymer flexibility on depletion interaction was studied in both isotropic and planar system via Monte Carlo computer simulation.

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Elastic properties of single particle systems: A molecular dynamics study

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We use the properties of free, spherical polymer brushes as a characterization of the shape of the spherical polymer brush; by using as a reference point the free brush, we implement an “up-bottom” linear elastic theory from the macroscopic to the microscopic case to describe the elastic properties of a single particle. By determining the elastic moduli of a microscopic object we obtain interesting physical insights on the properties of a single particle, e.g. we discover that upon uniaxial compression by parallel walls, the ratio of the relative transverse dilation measured at waist and the relative indentation depends on indentation. Due to the radial inhomogeneity on the microscopic level, these ratios appear to be dependent on the compression strength. The dilation-indentation ratios of the polymer brushes studied have values in the physically reasonable interval for isotropic and homogeneous macroscopic materials for a broad range of parameters. An important result of our study is that the ratios, we obtained approximately overlap for various number of chains, when scaled by the radius of gyration of the force-free brush. This indicates that the elastic properties of these microscopic particles are mainly independent of their actual internal structure and scale mostly with their equilibrium size. The results do not depend on the explicit wall-monomer interaction potential used. This conclusion is

supported by classical continuum elasticity calculations, where the finite-element method is used to minimize the energy and to find the displacement field. A simple hard-core soft shell model with constant Poisson ratios of the soft shell is used, and shows agreement with the simulation results for the elongation-indentation quotients for all indentations. Furthermore, comparison of the results with self-consistent field calculations shows semi-quantitative agreement.

Melting of colloidal molecular crystals on triangular lattices

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Studies of two-dimensional colloidal systems in the presence of two-dimensional external potential have revealed interesting ordering phenomena with counterintuitive reentrant phase behavior. The potential patterns have been produced by interfering laser beams and enabled systematic studies by smooth and controlled variation of the lattice constant and the strength of the external potential. Interesting phenomena arise when there are an integer number of colloidal particles per potential minimum. We propose a theory for the phase behavior of such two-dimensional colloidal systems in commensurate external potentials. The key idea is to reduce the problem to the low energy degrees of freedom by considering the integer number of colloidal particles which gather in a single potential minimum as a rigid composite object. We focus on the case of dimers and trimers on a triangular lattice. The resulting phases and phase transitions are discussed as a function of temperature and experimental control parameters. Monte Carlo simulations corroborate our analytical approach and are in very good agreement with the melting scenario of experimental findings.

Dynein – a giant making tiny steps in our cells

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Dynein is a huge molecular motor, i.e. a protein molecule that converts chemical energy stored in the ATP molecule to the mechanical work. It is involved either in the collective motion which produces rhythmic beating of cilia and flagella, axonemal dynein, or in the transport of cargo along the microtubule filaments towards cell nucleus, cytoplasmic dynein. Due to its large size and complexity the molecular mechanism of dynein motility has been poorly understood. In the last few years, the advances in different experimental techniques enabled studies on a single molecular level and revealed many details in structure and functionality. The gained knowledge facilitates better insights in the mechanism of the energy transduction from this motor and allows for the first comprehensive theoretical studies. We propose a mechano-chemical model for a processive motion of a single dimeric molecule of the cytoplasmic dynein. It is based on a study of an elastic analog of the complex molecule, consisting of a small number of basic elements. We determine in thermal equilibrium the bending conformations of the motor in various states, depending on the state of the hydrolysis of ATP and relative position of its binding sites to the microtubules track. The results are then implemented into the kinetic model. Using stochastic simulations we relate properties of the stepping to the elastic and kinetic parameters.

Crystallization close to the glass transition: Dynamic heterogeneities do not precede crystallization

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We address the question whether a crystallization event can be predicted based on observations of spatial variations in the mobility of a supersaturated melt. We have carried out computer simulations of overcompressed suspensions of hard monodisperse ellipsoids and observed their crystallization dynamics. The system was compressed very rapidly in order to reach the regime of slow, glass-like dynamics. We find that although particle dynamics become subdiffusive and the intermediate scattering function clearly develops a shoulder, crystallization proceeds via the usual scenario: Nucleation and growth for small supersaturations, spinodal decomposition for large supersaturations. In particular, we compared the mobility of the particles in those regions where crystallization set in with the mobility in the rest of the system. We did not find any signature in the dynamics that pointed towards the imminent crystallization event. Dynamic heterogeneity did not precede crystallization.

Geometrical frustration of chiral ordering in cholesteric droplets

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Confined chiral liquid crystals possess interesting optical properties that could be used as possible mechanisms to envisage soft matter optic and photonic elements in all-photonic circuits. The examples include spherical Bragg resonators [1] – cholesteric liquid crystal droplets which are characterised by tunable periodic modulations of refractive index. Here, we study cholesteric liquid crystal droplets, where the constraints induced by spherical confinement and chiral twisting of the liquid crystalline orientational order are crucial for the complexity of stable and metastable structures [2]. Detailed analysis of the droplet structures has shown presence of both cholesteric singular (τ) and non-singular (λ) disclinations in either double-helix like structures, loops or diametrical lines. Changing the intrinsic twisting of the molecular optical axes induces remarkable changes in the droplet structure and stability, modifying optical and photonic properties of the droplets. Depending on nematic anchoring at the confining spherical surface and on chirality numerous stable and metastable structures can occur. Our numerical simulations based on the minimisation of the Landau-de Gennes tensorial free energy yield more structures and more details not seen in director based modeling [3].

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Efficient simulation of colloidal dynamics in multicomponent fluids

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The recent development of micro- and nanofluidics has witnessed the versatility of multiphase and multicomponent fluids, for example in the high-speed, high-precision generation of droplets with controlled amount of solute. Simulating these systems in an efficient way is a complicated task, as they present several, well-separated spatial and temporal timescales. Here we present a novel computational method, based on the lattice-Boltzmann technique, that allows to simulate in an efficient way the dynamics of colloids in complex, multicomponent fluids. Several examples of the dynamics of neutral and charged colloids in pressure-driven flows characterized by moving contact lines are presented.

On possible existence of hydride nanoparticles in electro-reduced water

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Studying electron properties of liquid water in the frame of band theory shows that its non-stoichiometric state is a very important tool for varying physical and chemical properties and changing its reduction-oxidation (redox) potential of clean liquid water and aqueous solutions. In this connection, Fermi level in band gap, as an effective energetic factor of non-stoichiometric liquid water, is the most convenient energy for monitoring and managing the redox potential. A hypo-stoichiometric state, H_2O_{1-z} , of liquid water is realized when the position of Fermi level is near the bottom of conduction band. This state can be realized by micro emulsifying gaseous hydrogen in aqueous solution or by electro-reducing a weak solution of sodium chloride and forming nanoparticles of sodium hydride, NaH, in catholyte. The hyper-stoichiometric state, H_2O_{1+z} , can be realized in shifting down Fermi level to the top of valence band by saturating water with oxygen nanobubbles or by electro-oxidising the weak solution of sodium chloride and forming nanoemulsion of hypochlorous acid, $HOCl$, in anolyte. The nanohydrides (nanoacids) as strong reducers (oxidizers) are quasi-stable in corresponding parts of electrolyzed aqueous solutions and effective means for managing the redox potential. Therefore it is important monitoring Fermi level online by precise sensor having the exact measuring characteristics.

Many-body contact repulsion of deformable disks

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We use a spring-and-plaquette network model to analyze the repulsion between elastic disks in contact. By studying various 2D geometries, we find that as disks approach the incompressibility limit the many-body effects become dominant and the disk-disk interaction is not pairwise additive. Upon compression, the disks undergo a transition from the localized to the distributed deformation regime accompanied by a steep increase of energy consistent with the onset of a hard core. These results shed new light on the structures formed by deformable objects such as soft nanocolloids.

Bonded boojum-colloids in nematic liquid crystals

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Topological defects play a key role in the interaction of colloidal particles in liquid crystals. They appear as a consequence of broken orientational order, and their distribution around the colloidal particles determines the symmetry of long-range interactions. Colloidal particles induce surface alignment of the nematic molecules. When the nematic is aligned parallel to the surface of the colloidal particle, two surface topological defects, commonly known as boojums, are nucleated at antipodal points. Here we show that these defects exhibit a rather complex structure that depends on the combination of the strength of the surface potential, the size of the colloidal particle, the temperature, and the liquid crystal elastic anisotropy. Moreover, we will show that structural transitions of the defects core also occur for interacting boojum-colloids at short distances. In particular, boojum-colloids can assemble into linear chains bonded by defects connecting neighboring particles, similar to what is observed in cholesteric liquid crystals.

Liquid at zero temperature: Network entropy defeats the crystal in patchy particles

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In a typical phase diagram, cooling down a liquid to sufficiently low temperature causes it to become metastable with respect to crystallization. Here, we introduce a simple model for patchy particles where, surprisingly, the liquid phase remains stable even in the zero-temperature limit. Hence, it is possible to continuously transform a diffusive liquid to a fully arrested (gel) state along an equilibrium route. The patchy particles under consideration here are based on the Kern-Frenkel model [1], with the additional limitation that each patch can only form a single bond, analogous to colloids functionalized by a limited number of DNA strands. As a result of this limitation, we can tune the flexibility of the bonds without increasing the maximum number of bonds a particle can form. We use computer simulations and free energy calculations to study the phase behavior for particles with four attractive patches each, and show that for sufficiently small patches (or inflexible bonds), the liquid phase becomes metastable with respect to a diamond crystal structure at low temperatures, as expected [2]. However, increasing the flexibility of the bonds increases the number of ways a disordered, fully bonded network of particles can be formed. We show that it is this configurational entropy that stabilizes the liquid phase with respect to the crystal phase, even at zero temperature, where a fully bonded tetrahedral network is formed. Finally, we use event-driven molecular dynamics simulations to investigate the change in dynamics in the fluid phase as the system is cooled. The self-diffusion slows down exponentially as the temperature

decreases, following an Arrhenius-like behavior that can be understood directly based on the number of broken bonds in the network.

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Nonequilibrium growth of patchy-colloid networks on substrates

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Patchy colloids with highly directional interactions are ideal building blocks to control the local arrangements resulting from their spontaneous self-organization. Here we propose their use, combined with substrates and nonequilibrium conditions, to obtain novel structures, different from those of equilibrium thermodynamic phases. By contrast to equilibrium, the non-equilibrium films exhibit a fractal structure (gel) and the film density is always lower than the bulk equilibrium liquid density of the optimal network (zero pressure). We investigate numerically the irreversible adhesion of different types of patchy colloids, namely, three- and two-patch colloids and Lisbon colloids, near attractive substrates, and analyze the fractal network of connected particles that is formed. The network density profile exhibits three distinct regimes with different structures: Surface layer, liquid film, and interfacial region. We characterize in detail the scaling properties for the three-patch colloids case, for both unrestricted and confined colloids. The size dependence is well described by a power law with an exponent consistent with diffusion limited aggregation. The adsorption of a mixture of three- and two-patch colloids is also considered. An optimal fraction of two-patch colloids is found where the total density of the film is maximized, in contrast to the equilibrium gel structures where a monotonic decrease of the density has been reported. Lisbon patchy colloids, with temperature dependent valence, provide exquisite control of bulk properties. At equilibrium a rich phase

diagram was found, with reentrant phase transitions [1]. With nonequilibrium conditions, structural properties change both at the surface layer and the liquid film. Near the surface, the densities of the first layers can be controlled through the distribution of patches and their interaction. We propose a growth mode diagram and characterize the liquid film density as a function of the Lisbon colloids parameters. As in equilibrium, Lisbon colloids outperform mixtures of patchy particles.

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Chemically propelled nanodimer motors

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The conversion of chemical energy into directed motion on the nanoscale is widespread in nature. Biological molecular motors, such as kinesin and ATPsynthase, play essential roles in the transport and synthesis biochemicals in the cytoplasm and in cell motility. In addition to these biochemical motors, synthetic molecular motors have been designed that use chemical, light, or other energy sources to perform directed motion. A class of synthetic motors has been constructed that does not depend on conformational changes for their operation. This class of motors includes electrochemically synthesized striped bimetallic nanorods and synthetic catalytic molecules tethered to inactive particles. A model for chemically powered nanodimers that perform directed motion has been developed. The nanodimer consists of a pair of catalytic and chemically inactive spheres, in general with different sizes and with a fixed internuclear separation. Dimers can be designed so that the directed motion along the internuclear axis occurs in either direction and is much larger than the thermal velocity fluctuations, a condition needed for such nanodimers to perform tasks involving targeted dynamics. Such synthetic chemically powered nanomotors often rely on the environment for their fuel supply. The propulsion properties of such motors can be altered if the environment in which they move is chemically active. Dynamics of self-propelled nanomotors in chemically active and inactive media will be discussed.

Topologically entangled structures in nematic colloids

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Frustration of nematic order by geometric constraints or by intrinsic chirality offers an attractive topological background. Nematic braids formed by disclinations entangling colloidal particles in thin layers of nematic liquid crystal are restricted by topological rules that can be applied to design complex soft materials. Experiments show a rich variety of knotted and linked defect structures which can be manipulated and reconnected by laser light. We present the classification of entangled disclination lines by self-linking number and demonstrate how to obtain any desired knot or link on large enough lattice of colloidal particles. We believe that our concept of the topological tailoring of materials can be extended to other soft matter and colloidal systems, featuring novel, topology-determined material properties.

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Biomimetic folding particle chains

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Our goal is to experimentally realize directed self-assembly in the form of self-folding of colloid strings. We are inspired by how the sequences of amino acids dictate the folded 3D structure of proteins. We aim at similar directed self-folding on the colloidal scale. Simulations suggest that the prerequisites are: (i) different isotropic (long-ranged) interactions and (ii) an attractive directional (patchy) interaction between the colloids. We use existing polymer chemistry, free polymer induced depletion interactions and liquid-interface scaffold chemistry to realize such interactions.

Understanding colloidal interactions induced by wetting phenomena

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The physics of a colloidal suspension is often studied by modeling the solvent, in which the colloidal particles are dispersed, as a homogeneous medium. If in many practical situations this assumption is justified, there are important cases when this breaks down. In particular, when the solvent inhomogeneities develop on length scales comparable with the distance between the colloids, they can give rise to non-negligible effective colloid-colloid interactions. At present, there is an increasing attention towards interactions for which, as for the celebrated critical Casimir forces, the strength and range can be tuned with the temperature in a reversible way. In fact, in most practical situations the colloid-colloid interactions one considers, like those determined by electrostatics and depletion phenomena, are controlled by means of the chemical composition, and are thus irreversible. Understanding how thermally reversible interactions work can potentially offer an extraordinary (and simple) tool for manipulating colloidal suspensions. Here we focus on effective colloidal interactions induced by wetting phenomena. These arise when one of the components of a binary solvent preferentially adsorbs on the surface of the colloids. When the solvent is close to the first-order demixing region (but not necessarily to criticality) the adsorption layer grows on long length scales, thus determining an effective interaction between the colloids with varying strength and range. Wetting phenomena have been studied since the late 1970s, but a quantitative analysis of their

effect in colloidal systems, particularly beyond the “two-slit” approximation, lacks. Working within the framework of density-functional theory, we develop a simple theory aimed at describing wetting-induced colloidal interactions in various geometries. We compare the predictions of our theory with more refined (and less flexible) theories, and determine their quantitative effect on colloidal suspension when compared to critical Casimir forces.

Optical properties of ferrofluids: Cobalt nanoparticles dispersed in organic solvents

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Ferromagnetic fluids (ferrofluids) are homogeneous colloidal dispersions of ferromagnetic nanoparticles dispersed in a liquid carrier. In ferrofluids large linear and circular optical anisotropy can be induced by applying relatively small external magnetic fields [1]. Because of that they are extensively studied for applications in optical technology as fast shutters, switches, tunable phase retarders, etc. We present a study of Faraday effect (induced optical activity) and Voigt effect (induced birefringence) in a composite material made of cobalt nanoparticles embedded in a dielectric liquid host. Nanoparticles have a diameter of approximately 10 nm and are in a monodomain ferromagnetic state. The volume fraction of nanoparticles is of the order of 10^{-5} . Faraday rotation angle is measured as a function of external magnetic field, varying the size and concentration of nanoparticles and the wavelength of light. A nonlinear dependence of optical rotation on magnetic field resulting from the reorientation of nanoparticles is observed. To analyse experimental results, an effective dielectric tensor of a composite material into which thermodynamic properties of the system are incorporated was constructed. The proposed approach enables quantitative determination of the magnetic moment and plasma

frequency of a single nanoparticle, and from this the size of an effective magnetic diameter of nanoparticles [2]. To describe induced birefringence one also has to consider chains of nanoparticles, despite of their concentration being very small. We show that in dilute solutions only dimers of nanoparticles need to be considered [3]. The induced birefringence is quadratic in volume fraction of dimers as opposed to the Faraday effect that is linear in volume fraction of nanoparticles.

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Non-equilibrium dynamics of a bilayer system of confined colloidal particles in a planar shear flow

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We perform computer simulations of a confined bilayer system of charged colloidal particles interacting via a combined soft-sphere and Yukawa potential. The system is driven from equilibrium by a planar shear flow. The model parameters are adjusted according to ludox silica particles, which we have previously studied under equilibrium conditions [1, 2]. As a framework for solving the equation of motion, we employ overdamped Brownian dynamics simulations. We investigate the impact of the shear flow and confinement on structure formation and focus on statistical properties such as translational symmetry order parameter and pair distribution functions. Furthermore we are interested in the emergence of the zigzag motion observed in experiments [3] and characterized by the spatial oscillations of layers. We hope that our results can be used as predictions for future experimental work.

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Micro-swimmers confined to a sphere

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In nature bacteria live in confined environments of micrometer range size but little it is known about the effect of confinement on microbial behavior. We have developed a high throughput method to confine motile bacteria to water droplets in oil that allows simultaneous analysis of droplets with various radii and various bacteria concentrations. We have systematically measured the radial density distribution function of a smooth-swimming mutant of *E. coli* inside the droplets. Our results show a transition driven by micro-swimmer density: At low concentrations the cells mostly accumulate at the water-oil interface while for higher swimmer concentrations this distribution gradually extends to the entire volume of the droplet. This new class of emulsions that encapsulate biologically active matter constitutes an ideal system for discovery of new physics and has potential applications in food, industrial biotechnology and biomedicine.

Phase behavior of colloidal monolayers on one-dimensional periodic light potentials

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Phase transitions of colloidal monolayers on light-induced substrate potentials have been demonstrated to provide novel insights into the phase behavior of two-dimensional systems on patterned surfaces. Due to the interplay of repulsive interparticle forces and their interaction with the substrate, interesting structures will form which are also observed in atomic systems. Here, we study the phase transitions of charged colloidal particles on arrays composed of periodic one-dimensional laser lines which are created by a scanned laser beam. The colloidal particles used are suspended in an organic solvent with low polarity that causes the formation of spontaneous hexagonal crystals of large lattice constants as compared to those formed in aqueous solutions. This fact provided a new regime where phase transitions are accessed for different periods of the light patterned substrates.

Mosaic two-lengthscale quasicrystals

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Over the past decade quasicrystalline order was reported in many soft-matter systems including dendrons and tetrablock terpolymers, and diblock copolymer and surfactant micelles, establishing soft quasicrystals (QCs) as an integral part of the field. The existence of QCs in fuzzy macromolecular micelles suggests that they must be induced by a generic mechanism rather by specific chemistry. The most evident common feature of micelles stemming from the open architecture is their softness but no direct link to quasicrystallinity has been established. We theoretically study two-dimensional hard disks decorated with square-shoulder repulsion mimicking, e.g. the soft alkyl shell around the aromatic core in dendron micelles. We find a coherent sequence of QCs with 10-, 12-, 18-, and 24-fold bond-orientational order, which originate from mosaics of triangular and rhombic tiles based on core-to-core and shoulder-to-shoulder packed particles. The two-lengthscale pair interaction responsible for the novel phases is much more transparent than quantum-mechanical theories of metallic-alloy QCs, and it suggests that quasicrystallinity may be related to universal packing principles applicable to a range of objects from atoms to macromolecular assemblies.

To the theory of magnetodeformation of ferrogels and ferroelastomers

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Ferrogels and ferroelastomers present compositions of colloidal magnetic nanoparticles in polymer materials. Low magnitudes of the ferrogel elastic modulus provide their significant deformation under the action of quite moderate magnetic fields. It opens promising perspectives of these systems application in many smart technologies. One of the principally important and unclear problems in the science on the magnetopolymer compositions is the question on the type (elongation or contraction in direction of applied magnetic field) of their magnetodeformation. Some experiments demonstrate contraction, whereas the other ones show elongation of the samples. The main goal of this work is theoretical and experimental study of the fundamental features of the ferrogels/ferroelastomer deformation under the action of homogeneous magnetic field. Depending on concentration of the particles and their magnetic moments, they either can be homogeneously distributed in the polymer matrix or form linear chains, branched nets, dense columns and other structures. Analysis shows that the type and amplitude of the deformation are sensitive to the internal spatial distribution of the particles. Our results demonstrate that the type of the deformation depends on the strength of the applied magnetic field, on the sample shape and concentration of the imbedded particles as well. All these factors must be taken into account at the interpretation of experimental results.

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