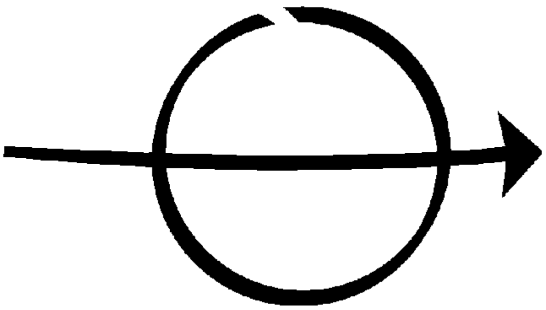
2nd International Conference

Colloidal Dispersions in External Fields

CODEF II



held on
31.03. - 02.04.2008
at the
Gustav-Stresemann Institut e.V. Bonn (Bad-Godesberg)

in conjunction with

Transregional Collaborative Research Centre SFB TR 6

Physics of Colloidal Dispersions in External Fields

Scope of the Conference

Soft matter in general and colloidal dispersions in particular are characterized by their susceptibility to manipulation by even weak external fields. The scientific focus of the conference is on the physics of colloids in confining geometries, under shear, as well as in electric, laser-optical and magnetic fields. Self-organization phenomena in equilibrium and non-equilibrium, where colloidal dispersions play a pivotal role as model systems, will be discussed. Particular emphasis will be put on the combined use of complementary methods, such as experiment, computer simulation and theory. The conference is held in conjunction with the Collaborative Research Centre **Transregio SFB TR6** "*Physics of Colloidal Dispersions in External Fields*". It is the second conference in a series that was started in 2004 by the CODEF I meeting. The number of participants in CODEF II (193 registrations from 19 different countries) has strongly increased as compared to that of the CODEF I meeting showing that colloids in external fields are a strongly growing research field.

Specific topics include:

- colloids in controlled nonequilibrium
- phase transitions induced by external fields
- dispersions in confinement
- real-space imaging and scattering
- theoretical models and simulation techniques

The scientific program includes also a poster session which is open to all participants.

Proceedings

The proceedings of the CODEF II conference will be published as a special issue of *Journal of Physics: Condensed Matter*.

Organizing Committee

K. Binder (Mainz), **A. van Blaaderen** (Utrecht), **J.K.G. Dhont** (Jülich), **S.U. Egelhaaf** (Düsseldorf), **M. Fuchs** (Konstanz), **K. Kremer** (Mainz), **H.N.W. Lekkerkerker** (Utrecht), **C.N. Likos** (Düsseldorf), **H. Löwen** (Düsseldorf), **G. Maret** (Konstanz), **P. Nielaba** (Konstanz), **T. Palberg** (Mainz), **D. Vollmer** (Mainz)

Local Organizing Committee

J.K.G. Dhont, S.U. Egelhaaf, S. Böhm, C.N. Likos, H. Löwen (Chair)

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- Sonderforschungsbereich TR6
- Johannes-Gutenberg-Universität Mainz, MWFZ
- Institute of Physics Publishing

Brief description of the Transregio SFB TR6:

Physics of Colloidal Dispersions in External Fields

The Transregio-Sonderforschungsbereich TR6 is focused on the rich **physics of colloidal dispersions**. The latter are solutions of mesoscopic solid particles with a stable (i.e. non-fluctuating) core embedded in a molecular fluid solvent. Among the various soft matter systems, colloidal dispersions play a prominent role as they can be both prepared and characterized in a *controlled way*. The effective interaction between the colloidal particles can be tailored by changing, e.g., the salt concentration in the solvent. Moreover, colloidal suspensions can be regarded as the simplest prototype of soft matter: the length scale separation between the molecular solvent and the mesoscopic particles is unique and complete. Spherical particles without any additional structure on the mesoscopic length scale possess the simplest and highest possible symmetry. This directly implies that a simple theoretical modeling of a single particle without many fitting parameters is possible. Exciting questions concern collective many-body effects induced by co-operation and self-organization of many particles. A striking advantage of colloidal dispersions lies in the fact that these questions can be studied simultaneously by using three different complementary methods, namely *experiment, computer simulation, and theory*.

A profound theoretical understanding also provides an insight into the general basic principles and mechanisms of phase transformations such that colloids play an exposed role as *model systems* for condensed matter in general. Colloids do play a similarly dominant role in exploring changes of soft matter properties **in external fields** which can be used to control the colloidal samples. This area is the central research topic in the Transregio-Sonderforschungsbereich SFB TR6.

There are two main streams of ongoing research: first colloidal suspensions serve as excellent model systems for controlled nonequilibrium situations where the control results from the field applied. Second, the shape and the internal degrees of freedom of the colloidal particles can get more and more complex. Correspondingly the response to an exposed field is more complex.

37 scientists from 5 locations (Konstanz, Mainz, Düsseldorf, FZ Jülich, and Utrecht) are carrying out collaborative research. The external fields can be:

A: shear fields

B: electric fields

C: laser-optical and magnetic

D: confining geometries

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CONFERENCE PROGRAM

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09:55 - 10:15	**A. Erbe, Universität Konstanz:** Lane formation in driven colloidal systems
10:15 - 10:35	**P. Keim, Universität Konstanz:** 2D colloidal model systems
10:35 - 10:55	*Coffee break*
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12:25 - 12:45	**M. C. Jenkins, Universität Düsseldorf:** Observation of colloidal suspensions in modulated light fields
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14:55 - 15:15	**K. Franzrahe, Universität Konstanz:** Field induced ordering phenomena and elastic properties in colloidal crystals
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10:15 - 10:35	**T. Schilling, Universität Mainz:** Depletion-induced phase transitions in suspensions of rod-like and spherical colloids
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11:30 - 11:50	**A. Imhof, Utrecht University:** Coarsening in colloid-polymer mixtures phase separating under shear
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12:25 - 12:45	**J. Stellbrink, Forschungszentrum Jülich:** Relating structure, dynamics and rheology of soft colloidal glasses
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12:25 - 12:45	**G.J. Vroege, Utrecht University:** Special magnetic behaviour of (modified) Goethite dispersions
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15:10 - 15:20	**S. U. Egelhaaf, Universität Düsseldorf: Closing remarks**

INVITED TALKS

T - 1

Model for assembly and gelation of four-armed DNA dendrimers

F.W. Starr,[2] J. Largo,[1] P. Tartaglia,[1] and F. Sciortino[1]
[1] *Dipartmento di Fisica e I.N.F.M., Universita di Roma "La Sapienza", Piazzale Aldo Moro 2, I-00185, Roma, Italy*
[2] *Department of Physics, Wesleyan University, Middletown, Connecticut 06459, USA*

I will discuss the phase diagram of a simple model for a dendrimeric particles functionalized by four single-strand DNA chains. The phase diagram of the system reveals analogies with the one of network forming liquids and the one expected for tetrehedrally coordinated patchy colloids. I will also show that developing an effective potential for particles interacting with a limited number of lock-and-key selective bonds (due to the specificity of biomolecular interactions) requires — in addition to the nonsphericity of the potential — a many body constraint that prevents multiple bonding on the same site. The effective potential exhibits a rich phase diagram that includes at least four thermodynamically distinct amorphous phases (polyamorphism) in a one-component system. The dense phases consist of a hierarchy of interpenetrating networks. This result demonstrates that bonding selectivity can provide an effective route to generate new networked materials with polyamorphic behavior. The interpenetration of networks provides an alternative simple, generic mechanism to understand the generation of multiple liquid phases, such as observed in phosphorus and expected to occur in water, silica, and several other network forming fluids.

[1] J. Largo, P. Tartaglia, and F. Sciortino, Effective nonadditive pair potential for lock-and-key interacting particles: The role of the limited valence, Phys. Rev. E **76**, 011402 (2007)

[2] J. Largo, F. W. Starr, F. Sciortino, Self-Assembling DNA Dendrimers: A Numerical Study Langmuir, **23**, 5896-5905. (2007)

[3] F.W. Starr, F. Sciortino Model for assembly and gelation of four-armed DNA dendrimers J. Phys. Cond. Matt. **18**, L347-L353, (2006)

T - 2

Lane formation in driven colloidal systems

A. Erbe, M. Zientara, and P. Leiderer
University of Konstanz, Department of Physics, D-78457 Konstanz, Germany

We investigate the formation of lanes in infinite 2-dimensional systems of colloidal particles. The particles are either binary mixtures of magnetic and non-magnetic particles, which are driven in opposite directions, or monodisperse systems of magnetic particles. The non-magnetic particles are driven by gravity; the magnetic particles can be either moved in a gradient of a magnetic field or by gravity as well. The origin for the formation of lanes is investigated. In a monodisperse system it most likely occurs due to hydrodynamic effects, while in binary mixtures lane formation due to slipstream effects can be expected. We show experiments on such systems and compare the results to Brownian dynamics simulations.

T - 3

2D colloidal model systems

P. Keim, F. Ebert, P. Dillmann, and G. Maret
University of Konstanz, Department of Physics, D-78457 Konstanz, Germany

In this talk results of two types of two-dimensional colloidal systems are presented. They consists of superparamagnetic colloidal particles confined by gravity to a flat water/air interface. By applying an external magnetic field perpendicular to the sample plane the repulsive dipole-dipole interaction between the particles and therefore the system temperature can be adjusted over a wide range. Video microscopy yields time dependent positions of several thousand particles on all relevant length- and timescales.

A system of colloids bi-dispersed in size and interaction strength shows typical features of a glass former. Decreasing temperature the system traverses from a fluid to a dynamically arrested state while staying amorphous. Although the system has no long range order and exhibits glassy dynamics, different types of stable crystallites are found locally. The local order is explained by a small set of specific crystal structures. The statistic of this crystal unit cells shows a continuous increase of local order with decreasing system temperature as well as a dependence on sample history and local composition.

A system of mono-disperse colloids solidifies at low temperatures into a hexagonal crystal. The two step melting scenario of Kosterlitz, Thouless, Halperin, Nelson, and Young (KTHNY-theory) with the intermediated hexatic phase is verified in detail. On the other hand performing a temperature quench out of thermal equilibrium the system solidifies by a nucleation process. The local bond order parameter is used to distinguish crystalline particles from those in the fluid. By tracking the crystalline regions over time we can investigate the nucleation process and the growth of colloidal crystallites in time.

T - 4

Simulation and theory of nanoparticles in liquid crystals

M.P. Allen and D.L. Cheung
Department of Physics and Centre for Scientific Computing, University of Warwick,
Coventry CV4 7AL, United Kingdom

Simple density functional calculations in the Onsager approximation have been used to calculate the position- and orientation-dependent single particle density of liquid crystals in the nematic and isotropic phases. The structure of the solvent around spherical and non-spherical nanoparticles, both in the bulk colloidal suspension and in the vicinity of walls, have been determined, along with the effective forces produced by these deformations. These results, and comparisons with Monte Carlo calculations, will be presented.

T - 5

Colloidal crystal growth at externally imposed nucleation clusters

S. van Teeffelen, C.N. Likos and H. Löwen
Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf,
D-40225 Düsseldorf, Germany

We study the conditions under which and how an imposed cluster of fixed colloidal particles at prescribed positions triggers crystal nucleation from a metastable colloidal fluid. Dynamical density functional theory of freezing and Brownian dynamics simulations are applied to a two-dimensional colloidal system with dipolar interactions. The externally imposed nucleation clusters involve colloidal particles either on a rhombic lattice or along two linear arrays separated by a gap. Crystal growth occurs after the peaks of the nucleation cluster have first relaxed to a cutout of the stable bulk crystal.

T - 6

Colloidal Gelation

D.A. Weitz
Department of Physics and Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138

This talk presents the results of a set of careful experiments to investigate the fundamental nature of the gelation of colloidal particles with an attractive interaction between them. Effects due to gravity are minimized to allow the underlying mechanisms to be studied. The results show that when the range of the interaction potential is small, all colloidal gelation is driven initially by spinodal decompostion. This includes the ultimate limit, diffusion-limited cluster aggregation, which has long been considered a purely kinetic process, but which is driven initially by a near-equilibrium process.

T - 7

Observation of colloidal suspensions in modulated light fields

M.C. Jenkins, S.U. Egelhaaf
Institut für experimentelle Physik der Kondensierten Materie (IPkM), Heinrich-Heine-Universität Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf, Germany

Colloidal systems often exhibit disorder-order transitions, sometimes counter-intuitively. Such transitions are seen across the spectrum of interparticle interactions, ranging from long-range to nearly-hard-sphere interactions, and can be explained on thermodynamic grounds. However, what occurs during crystallisation, in which a system acquires order at well-defined wavevectors, still poses interesting questions. Furthermore, sometimes the expected order transition does not occur and the systems remains in a disordered glass state, an intriguing dynamically arrested state.

To investigate the emergence or otherwise of order at specific wavevectors, we are interested in the respose of a system to stimuli at those and other wavevectors. Accordingly, we use periodically modulated light fields–essentially structured optical tweezers–to generate the necessary external potential. To obtain local information on the response, we track particles in real space by optical microscopy.

T - 8

Glassy colloids in shear fields

J.-L. Barrat
Laboratoire de Physique de la Matière Condensée et Nanostructures, Universite Claude Bernard - Lyon I,

I will discuss some aspects of flow in glassy systems that have been investigated recently using computer simulations. I will start with a description of elastic and plastic deformations at zero temperature (“athermal” systems), in which case it is possible to decompose the deformation in terms of elementary plastic events. I will also discuss some statistical properties of homogeneous flow in glassy systems at finite temperature using the “effective temperature” concept. Complex phenomena such as yield stress, shear banding, complex stress strain curves, commonly in colloidal pastes, can be observed place in a very simple “computer glass” model. The existence of shear bands can be understood from the presence of a nonzero yield stress, larger than the small shear limit of homogeneous flow curves. This in turn implies that the flow curve is effectively nonmonotonic, and allows shear band formation in a restricted domain of shear rates. Finally, I will present some recent results concerning shear induced crystallisation.

T - 9

Colloidal interactions at interfaces - electrostatics, capillarity and fluctuations

M. Oettel
Institut für Physik der Kondensierten Materie (KOMET), Johannes Gutenberg Universität, 55128 Mainz, Germany

The effective interaction of colloids trapped at fluid interfaces exhibit qualitatively new features when compared to the ones in colloidal bulk solutions. First, electrostatic interactions which are exponentially screened in ionic solvents become multipolar, longer–ranged at interfaces between water and a nonpolar medium (usually taken to be air or oil). Regardless of the details of the charge distribution on the colloids, the leading multipole is always a dipole oriented perpendicularly to the interface [1]. We show (within Poisson-Boltzmann theory) that charge renormalization makes this effective dipole weakly dependent on the surface charge density on the water side and independent on the salt concentration in the high charge density limit [2]. This is in stark contrast to expectations from linear Debye-Hückel theory which has been used frequently to interpret experimental results. Secondly, capillary interactions mediated by deformations of the interface can be expected to dominate the electrostatic interactions for anisotropic colloids. The example of ellipsoidal colloids is discussed [3]. Thirdly, capillary wave fluctuations lead to a fluctuation induced force between the colloids (thermal Casimir effect) whose range strongly depends on the boundary conditions determining the three-phase contact line. The colloidal shape is reflected in the anisotropy of the resulting fluctuation interaction as the comparison between spherical and ellipsoidal particles shows [3].

[1] A. Dominguez, D. Frydel, and M. Oettel, Phys. Rev. E (R) (in print).

[2] D. Frydel, S. Dietrich, and M. Oettel, Phys. Rev. Lett. **99**, 118302 (2007).

[3] E. Noruzifar, H. Lehle, and M. Oettel, Eur. Phys. J. E (submitted).

T - 10

Field induced ordering phenomena and elastic properties in colloidal crystals

K. Franzrahe
Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Minimization trends in physics and technology have caused a lot of interest in monolayers, their interactions with a substrate and the influence of confinement lately. Colloidal suspensions have proven to be ideal model systems for studies on such systems. The question of how the addition of another length scale into such a system will influence the intricate competition between adsorbate-adsorbate interaction and adsorbate-substrate interaction is addressed by studying a binary 50% mixture under the influence of a 1D spatially periodic substrate potential [1]. The interaction with the substrate completely changes the miscibility of the binary mixture. In addition such a system exhibits a field induced ordering transition and a so called fissuring regime. We show that these phenomena are to be found even in purely repulsive systems as a 2D hard disk mixture by means of Monte Carlo computer simulations.

Further research within the SFB-TR6 project section C4 concern generic effects of confinement on crystalline order in 2D systematically analyzed via Monte Carlo computer simulations and the elastic properties of fcc crystals consisting of charge stabilized colloids as determined from real space imaging experiments using confocal microscopy. Detailed information will be given on a separate poster of project section C4.

[1] K. Franzrahe and P. Nielaba , Phys. Rev. E 76, 061503 (2007)

T - 11

Interactions and dynamics of defects in colloidal crystals

C. Dellago
Institute for Experimental Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria

Using computer simulations, we investigate the structure and dynamics of point defects in colloidal crystals. In particular, we study how the effective interactions of defects determined in simulations can be rationalized in terms of elastic continuum theory. In a system with multiple defects, one finds attractive interactions both for vacancies and interstitials. Such attractive interactions, leading to defect clustering and observed also in irradiated metals, occur for various interaction potentials with a strength that depends on thermodynamic conditions and on the structure of the underlying lattice. While elasticity theory properly describes the disturbances and interactions created by lattice imperfections on a larger scale, defect interactions on spatial scales of the order of a few lattice constants are essentially determined by discrete lattice effects. Due to the long-range nature of the lattice distortions caused by defects, a comparison of simulation results with continuum theory requires the application of appropriate boundary conditions, which can be handled, for instance, with Ewald-summation.

T - 12

Cooperative lengthscales in glass-formers

J.-P. Bouchaud
CEA–Service de Physique de l’Etat Condensé, Centre d’Etudes de Saclay, 91191 Gif-sur-Yvette, France

Glasses are often described as a bona fide state of matter. The aim of this talk is to review several ideas, old and new, about what makes glasses so special as a state of matter: glasses are liquids that do not flow, characterized by increasingly cooperative dynamics.

T - 13

Simulating Entropic Gels

D. Frenkel[1,2] and B.Bozorgui[1]
[1] *FOM Institute for Atomic and Molecular Physics, University of Amsterdam, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands*
[2] *Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom*

I will discuss numerical simulations and simple theories to describe the phase behaviour of colloids coated by single-stranded DNA of varying length. We find evidence for an entropic phase transition, similar to the one predicted by A. Zilman et al (PRL 91, 015901 (2003)) on the basis of mean-field theory. The simulation suggest that this phase transition is kinetically arrested. This conclusion is supported by recent experiments.

T - 14

Crystalline structures in two-dimensional binary colloidal mixtures

R. Messina
Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf,
Universitätsstr. 1, 40225 Düsseldorf, Germany

It is well known that two-component mixtures exhibit much richer crystallization phenomena and polymorphism than their one-component counterparts. Tailoring the colloidal composite structures may lead to versatile materials such as photonic layers or molecular sieves. Consequently understanding how the phase behavior in mixtures depends on the interparticle interaction is motivated by fundamental as well as practical reasons. In this talk, the phase diagram of binary mixtures of particles interacting either via (i) a screened Coulomb potential [1] or (ii) a pair potential of parallel dipoles [2] is presented. Using lattice sums, a rich variety of stable crystalline structures of the type $A_m B_n$ are detected. Similarities and discrepancies of the phase behavior stemming from different type of inteparticle interactions (dipolar, screened Coulomb, hard disk) are discussed.

[1] L. Assoud, R. Messina and H. Löwen, cond-mat arXiv:0801.1453

[2] L. Assoud, R. Messina and H. Löwen, Europhys. Lett. 80, 48001 (2007)

T - 15

Fun with colloid-polymer mixtures, quenched disorder, and placing brackets

R. Vink
Institute of Theoretical Physics, Georg-August-Universität, Friedrich-Hund-Platz 1,
D-37077 Göttingen, Germany

Mixtures of colloids and polymers are interesting model systems. Even more interesting is when such a mixture is placed inside a random matrix of immobile (quenched) particles. In addition to the conventional thermal average, properties of interest now also involve an average over different disorder realizations. It then becomes possible to construct quantities like $[\langle x \rangle^2] - [\langle x \rangle]^2$, where $\langle . \rangle$ denotes the thermal average, and $[.]$ the disorder average. In the absence of quenched disorder, such a quantity would be trivially zero, but in the presence of disorder, this need not be so. In fact, in this presentation, I will provide simulation evidence for the existence of a divergence in one such quantity, and uncover an important link to the random-field Ising model.

Note also the POSTER version of this presentation (P-113)

T - 16

Depletion-induced phase transitions in suspensions of rod-like and spherical colloids

T. Schilling
Institut für Physik, Johannes Gutenberg Universität, 55099 Mainz, Germany

When non-adsorbing polymers are added to an isotropic suspension of rod-like colloids, the colloids effectively attract each other via depletion forces. We performed Monte Carlo simulations to study the phase diagram of such rod-polymer mixtures.

Large amounts of depletant cause phase separation of the mixture. We estimated the phase boundaries of isotropic-isotropic coexistence both, in the bulk and in confinement. To determine the phase boundaries we simulated in the grand canonical ensemble using “successive umbrella sampling” and we performed a finite-size scaling analysis to estimate the location of the critical point. The results are compared with predictions of the free volume theory developed by Lekkerkerker and Stroobants [Nuovo Cimento D **16**, 949 (1994)]. We also give estimates for the interfacial tension between the coexisting isotropic phases and analyse its power-law behaviour on approach of the critical point.

T - 17

Polymeric globules and coils: shear and sedimentation effects

R. R. Netz
Physics Department, Technical University Munich, 85748 Garching, Germany

The dynamics of globular and coil-like polymers under shear or sedimentation differs in some important aspects from hard colloids. This is so because polymers exhibit visco-elasticity on various time and length-scales and because configurational fluctuations are thermally activated. Such questions combine the fields of non-equilibrium thermodynamics, elasticity theory and hydrodynamics. Theoretical approaches thus rely on a combination of molecular simulations, continuum modeling and scaling approaches. This is demonstrated with a few examples:

i) The shear-flow induced unfolding of proteins plays an important role in starting the coagulation cascade in small blood vessels. In the theoretical modeling the unfolding is initiated by single-chain protrusion-like excitations and leads to a hydrodynamic unfolding transition, which is well captured by a scaling nucleation argument[1-3].

ii) Flexible polymers in strong sedimentation fields are subject to internal recirculation flows, which lead to compaction; for even larger sedimentation velocities, stretching into a hydrodynamically stabilized tad-pole structure occurs. The resulting sedimentation coefficient shows anomalous behavior[4].

[1] “Shear-Flow-Induced Unfolding of Polymeric Globules”
A. Alexander-Katz, M.F. Schneider, S.W. Schneider, A. Wixforth, and R.R. Netz
Physical Review Letters, **97**, 138101 (2006)

[2] “Shear-induced unfolding triggers adhesion of von Willebrand factor fibers”
S.W. Schneider, S. Nuschele, A. Wixforth, C. Gorzelanny, A. Alexander-Katz, R.R. Netz, and M.F. Schneider
PNAS **104**, 7899 (2007)

[3] “Surface-enhanced unfolding of collapsed polymers in shear flow”
A. Alexander-Katz and R. R. Netz
Europhysics Letters **80**, 18001 (2007)

[4] “Anomalous Polymer Sedimentation Far from Equilibrium”
X. Schlagberger and R.R. Netz
Physical Review Letters **98**, 128301 (2007)

T - 18

Coarsening in colloid-polymer mixtures phase separating under shear

A. Imhof
Soft Condensed Matter, Debye Institute, Utrecht University, The Netherlands

We study phase separation of a colloid polymer mixture in the spinodal two phase region of the phase diagram in shear flow. A counter rotating shear cell is used to image the system with confocal laser scanning microscopy. The system is quenched from an initially almost homogeneous state at very high (200 s^{-1}) shear rate to a low shear rate $\dot{\gamma}$. Initially, a spinodal decomposition pattern is observed. Its characteristic length scale increases linearly with time. As the structure coarsens, shear begins to impose a certain length scale onto the structure. The domains become highly stretched along the flow direction, and the domain size along the vorticity axis reaches a stationary size, which scales as $\dot{\gamma}^{-1/3}$. Furthermore, by quenching from an intermediate (6.7 s^{-1}) to a low shear rate the elongated structures become Rayleigh unstable and break up into smaller structures. However, the system eventually reaches the same steady state as was reached through coarsening in a direct high-to-low shear rate quench.

T - 19

The Simulation of Flow of Colloids and Polymers by Non-equilibrium Molecular Dynamics

I. Snook
Applied Physics, School of Applied Sciences, RMIT University, Melbourne, Australia

One of the most easily observed and most studied cases of an external field acting on a colloidal dispersion is that due to a fluid flow. Many fascinating phenomena have been seen in such systems and their practical importance is enormous in fields such as processing and transport of materials. Simulation of these systems by traditional Brownian Dynamics (BD) methods is made complicated by wall effects and in particular the need to include complicated many-body configuration dependent hydrodynamic interactions between the particles and between the particles and the walls. A further complication also arises from having to find an appropriate choice of boundary conditions at the wall. In order to study such phenomena and to provide data to test BD simulations we have made Non-equilibrium Molecular Dynamics (NEMD) simulations of the flow of colloidal and polymer particles in a thin channel with explicit inclusion of the background fluid. These simulations used atomic walls which were thermostated and the imposition of an external field to produce planar Poiseuille flow at low Reynolds number. Results will be presented to show the effect of channel width and flow rate on the velocity, density and temperature profiles. For wide channels these profiles are in agreement with the results of macroscopic fluid dynamics but discrepancies start to appear when the channel widths become smaller until finally the profiles are dominated by wall effects such as particle layering and then macroscopic theory is not even qualitatively correct. Also it is observed that colloidal particles tend to migrate to the walls but the polymer solutions simulated here tend to migrate to the centre of the channel.

T - 20

Relating structure, dynamics and rheology of soft colloidal glasses

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Soft colloids are the link between colloids and polymers, showing some unique features resulting from this special hybrid character. Recently, regular star polymers and block copolymer micelles have been independently used to investigate structure, dynamics and rheology on approaching the glass phase as a function of softness.

For kinetically frozen (PEP_m-PEO_n) block copolymer micelles we have shown, that the architecture of the individual micelle can be adjusted between the limits compact sphere like ($m \approx n$) and star-like ($m \gg n$). At the same time the (repulsive) micellar interactions vary from hard sphere like to ultra soft. Micellar structure factors in equilibrium can be described starting from either the hard sphere or the ultra-soft pair potential without adjustable parameters. Therefore PEP-PEO micelles are an excellent model system for soft colloids. Special emphasis will be on non-equilibrium phenomena as i.) jamming transitions in concentrated micellar solutions as observed by dynamic light scattering, pfg-nmr and rheology and ii.) the structural response of ordered/disordered colloidal phases to applied external shear as resolved by in situ neutron scattering techniques (Rheo-SANS).

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[3] M. Laurati, J. Stellbrink, R. Lund, L. Willner, D. Richter, and E. Zaccarelli, *Phys. Rev. E*, **76**, 041503, 2007.

T - 21

Dynamics of colloidal particles suspended in complex fluids: Fluid particle dynamics simulation study

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Liquid suspensions containing colloids are of fundamental importance in soft matter physics, colloid chemistry, and biorheorogy. For example, interactions between colloids often include an attractive part, which leads to the formation of colloidal aggregates. Such phenomena strongly affect the rheology of suspensions. To understand these phenomena, it is crucial to properly take hydrodynamic interactions among colloidal particles into account. However, hydrodynamic interactions between particles are quite difficult to deal with, because of the long-range nature and the resulting strong nonlocal couplings among all the relevant degrees of freedom of colloidal suspensions. To get rid of this difficulty, we proposed a new simulation method [Fluid Particle Dynamics (FPD) method]. In this method, liquid molecules are treated as a continuum fluid. The key feature is to regard a solid colloidal particle as an undeformable fluid one of high viscosity; i.e., we assume that viscosity changes smoothly across the interface between the inner and the outer region of each particle. This makes us free from the solid-fluid boundary condition, which is the origin of all the difficulties. Since in our FPD method all the degree of freedoms such as the particle distribution and the velocity field can be described by field variables, it is quite straightforward to incorporate new field variables such as charges, orientational order, and concentration fields. Here we apply the FPD method to understand the aggregation process of colloidal particles interacting with a Lennard-Jones potential, the dynamics of charged colloidal suspensions, and the dynamics of colloidal particles immersed in a critical binary mixture, and a nematic liquid crystal. We discuss interesting phenomena, which are caused by dynamic couplings between colloid motion and additional degrees of freedom in the surrounding complex liquids through the flow field.

This work was done with collaboration with Kumiko Kamata and Takuya Suganuma.

T - 22

Colloids in AC fields: Edge localized instabilities in dielectrophoretic bottles

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Dielectric colloids dispersed in a dielectric liquid experience a body force in gradients of AC fields. This force is due to the contrast in the dielectric properties between the colloids and the surrounding liquid. It allows to tune the concentration of colloids in the dielectrophoretic bottle by changing the applied field. We investigate the process of filling the dielectrophoretic bottle, i.e., directly after turning the field on. Our system consists of sterically stabilized PMMA colloids in a densitymatching mixture of decaline and cyclohexyl bromide. At high frequencies of the applied field (100 kHz to 1 MHz), we find that the spatially homogeneous migration of the colloids can be unstable against localized colloidal flows. Our experiments indicate a critical value of the driving force for the instability. The onset is at a field of $\approx 0.5V/\mu m$ in the dielectrophoretic bottle. We analyze this instability in analogy to the Rayleigh-Taylor instability. In contrast to the standard Rayleigh-Taylor instability, the driving body force is not due to gravity but due to the applied field gradient.

T - 23

Hydrodynamic and electrokinetic effects on the dynamics of charged colloids and macromolecules

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We explore dynamic processes in suspensions of charge-stabilized colloidal particles and macromolecules. Various transport properties like diffusion coefficients and viscosities, and dynamic scattering functions have been calculated using a many-component mode-coupling theory adapted to Brownian particles with hydrodynamic interactions, and by means of a recently developed accelerated Stokesian Dynamics simulation tool. Results obtained from theory and simulations are compared with static and dynamic scattering experiments on colloidal spheres and biological macromolecules. Salient results of this study comprise the absence of screening of hydrodynamic flow in salt-free fluid suspensions, the influence of the electrolyte ion kinetics on the colloid diffusion in non-dilute systems, and a hydrodynamic explanation for the unexpected non-monotonic concentration dependence of long-time self-diffusion observed in dispersions of DNA fragments. Furthermore, we analyze the validity of generalized Stokes-Einstein relations, and we point to the distinctly different behavior of low-salt charge-stabilized systems in comparison to suspensions of neutral hard spheres.

T - 24

Computer simulations of colloidal electrophoresis

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The “raspberry” model for colloidal particles is used to study electrophoresis of charge–stabilized colloidal dispersions. This model comprises a stochastic lattice Boltzmann background to take into account hydrodynamic interactions, and a system of point particles simulated via stochastic Molecular Dynamics. The parts are coupled via Stokes–like dissipative forces. A colloidal sphere is modeled via a large central particle enclosed by a two–dimensional network of small particles. Ions are taken into account as explicit small particles. It is argued that, due to hydrodynamic screening, a single–colloid simulation gives a good approximation to the behavior at the corresponding finite volume fraction. The electrophoretic mobility is obtained via non–equilibrium simulations, and Green–Kubo integration. The electrophoretic mobility is analyzed in terms of dimensional analysis. It is shown that a system of colloids plus counterions (without added salt) must be described in terms of four dimensionless scaling variables, of which two are identified as particularly relevant. Furthermore, effective parameters are introduced by means of standard charge renormalization. Within this theoretical framework, good agreement between the simulation data and Doppler velocimetry experiments in the low–salt regime can be obtained.

T - 25

Finite particles systems in strongly coupled dusty plasmas

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Particle-containing (dusty) plasmas are ideal systems to study effects of strong coupling where the electrostatic interaction between neighboring particles by far exceeds their thermal energy. In dusty plasmas, microspheres are trapped in a gaseous plasma. There the particles attain a high negative charge due to the continuous inflow of plasma electrons and ions. Due to this high charge the particles can crystallize into ordered structures. The size and time scales of these systems allow a detailed observation by video microscopy.

Recently, dust systems with a small, finite, number of particles have attracted growing interest because of their interesting properties. For dust clusters the boundary imposed by the confinement plays a crucial role. As a consequence, the structure of dust clusters drastically depends on the exact particle number N. Simultaneously, the dynamic properties of dust clusters show a strong dependence with particle number.

In this talk, the fundamental properties of finite and extended dusty plasmas are presented. Recent progresses in diagnostic techniques are described which allow to reveal fundamental properties of dust clusters. The structure and the fascinating interplay of structure and dynamical properties will be demonstrated for dust clusters in 1D, 2D and 3D confinement potentials.

T - 26

The phase behavior of attractive rod-like viruses under shear flow as studied by Small Angle Light Scattering

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The phase behavior of a dispersion of rods is strongly effected when this dispersion is subjected to a shear flow. Here we present the full non-equilibrium phase diagram for rod-like viruses (fd) with a depleting polymer as determined by Small Angle Light Scattering. We show that the binodal, which gives the shear rate and concentration where the dispersions becomes meta-stable, is influenced by the tumbling-flow aligning transition of the rods. The spinodal, which gives the shear rate and concentration where the dispersions becomes unstable, goes to lower concentrations with increasing shear rate. The maximum of the binodal $\dot{\gamma}_{max}$ is located at a much higher shear rate than the maximum of the spinodal and increases with increasing attraction. The shape of this non-equilibrium phase diagram does not depend on the attraction between the rods, when the diagram is scaled to the $\dot{\gamma}_{max}$ and the equilibrium binodal points.

T - 27

Mesoscale hydrodynamics simulations of attractive rod-like colloids in shear flow

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Suspensions of rod-like colloids with attractive interactions show in equilibrium an isotropic-nematic coexistence region, which widens with increasing interaction strength. We study the behavior of this system in shear flow. A hybrid simulation approach is employed, which consists of a mesoscale particle-based hydrodynamics technique (multi-particle collision dynamics) for the solvent and molecular dynamics simulations for the colloidal rods [1,2]. In shear flow, the system remains phase-separated below a critical shear rate, which increases with increasing attraction. Alignment and densification are induced by the flow in the isotropic phase, while the nematic phase shows a collective rotation motion. The difference of densities between these two regions allows us to determine the binodal lines. Our simulation results are compared with experimental results for suspensions of rod-like viruses.

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T - 28

A binary Yukawa mixture under shear: A computer simulation study of the transient dynamics

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Various experiments and computer simulations have demonstrated that shear strongly affects transport properties of glassforming liquids. If the shear rate exceeds the typical relaxation time of the system, an acceleration of the dynamics is observed which is reflected, e.g., in a decrease of the shear viscosity (shear thinning). The underlying mechanism of this change is still not well understood on a microscopic level. Recently, Fuchs and Cates [Phys. Rev. Lett. 89, 248304 (2002)] have developed a mode coupling theory (MCT) for glasses and liquids under shear where the steady state is derived through an integration over the transient dynamics. In order to check the latter MCT on a fundamental level we study the transient dynamics of a glassforming Yukawa liquid under shear by extensive molecular dynamics computer simulations. On the one hand, the dynamics from equilibrium to steady-state is considered, after a constant shear field has been switched on. On the other hand, we study the dynamics from the steady-state back to equilibrium. In both cases, the dynamics is analyzed by various quantities such as mean-squared displacements, time-dependent density correlation functions and the stress-strain relation. A rich phenomenology is observed. For the transition from steady-state to equilibrium, we demonstrate that, at least on a qualitative level, MCT is able to correctly reproduce the stress-strain relation as seen in the simulation.

T - 29

Hypersonic phononic colloidal crystals

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Soon after the birth of the photonic crystals with periodic variations of dielectric constant, theoretical and experimental work embarked on the propagation of acoustic waves in structures with periodic variations of density and/or sound velocities. The experimental realization of phononic crystals was up to now restricted to manually fabricated structures with macroscopic spacing and hence band gaps in the sub MHz frequency range. In contrast to the sonic and ultrasonic crystals, the study of hypersonic crystals at the submicron scale imposes substantial demand on fabrication and characterization techniques, which are currently being developed.

The dispersion of high frequency (GHz) acoustic excitations in three-dimensional colloidal crystalline or amorphous assemblies of sub-micron colloidal particles in different matrices was measured by high resolution Brillouin light scattering (BLS) in order to explore the phononic and elastic properties of nanostructured materials. In air, we record eigenmodes of the individual particles, which are shown to be independent from the crystallinity and the composition of the sample but sensitively depend on the particle architecture (e.g core/shell silica/poly(methylmethacrylate), hollow spheres) and their mechanical properties at nanoscale. In fluid matrices, the dispersion relation between the frequency and the wave vector ($k_{||}$ parallel to the fcc (111) plane) of the thermally excited acoustic waves has revealed two hypersonic phononic band gaps of different nature: (i) a Bragg gap occurring at the boundary of the first Brillouin zone and (ii) a hybridization-gap resulting from the interaction of particle eigenmodes with the acoustic mode of the effective medium. The hybridization gap is robust against structural disorder while disorder eliminates the Bragg gap. Depending on the particle size and the speed of sound in the infiltrated fluid, the frequency and the width of the hypersonic phononic c gaps can be tuned.

Since hypersonic crystals can simultaneously exhibit phononic and photonic band gaps in the visible spectral region, the technological applications could range from tunable filters and heat management to acoustic-optical devices.

T - 30

Constitutive equation for colloidal suspensions

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We present a first principles approach to the rheology of dense colloidal suspensions subject to homogeneous but otherwise arbitrary flow. Starting from the fundamental Smoluchowski equation for interacting Brownian particles neglecting hydrodynamic interactions we derive exact results for calculating time dependent averages, which lead e.g. to a generalized Green-Kubo relation for the stress tensor. Using Mori-Zwanzig type projection operator steps we develop a formally exact equation of motion for the transient density correlator which captures structural relaxation under flow. Approximations to these quantities are then developed which lead to a general constitutive equation for dense dispersions under arbitrary homogeneous flow. As the approximations used are tailored to treat high density systems our final equations allow the time dependent rheology of glassy colloidal suspensions to be investigated. We demonstate the effectiveness of our approach by presenting numerical results for shear [1] and general flows, including step-strain/compression, steady-shearing and creep.

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T - 31

Phase field approach to polycrystalline solidification including heterogeneous and homogeneous nucleation

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The phase field approach is applied to describe homogeneous and heterogeneous crystal nucleation in undercooled melts. The height of the nucleation barrier is determined by solving the appropriate Euler-Lagrange equations. The examples to be shown include homogeneous crystal nucleation in the hard-sphere fluid [1] and crystal nucleation in the liquid miscibility gap of a eutecticalloy [2]. In addressing heterogeneous nucleation, the foreign surfaces are defined via boundary conditions that realize the prescribed contact angle at the wall-crystal-liquid triple junction, as discussed in Ref. [3]. Finally, the phase field method will be applied for modeling crystalline solidification in 2D and 3D. The thermal fluctuations that lead to homogeneous and heterogeneous nucleation are included by adding fluctuation-dissipation noise to the governing equations. Simulations showing nucleation of complex surfaces will be presented (for a few examples see Fig. 1). Difficulties that complicate quantitative simulations of nucleation will be outlined.

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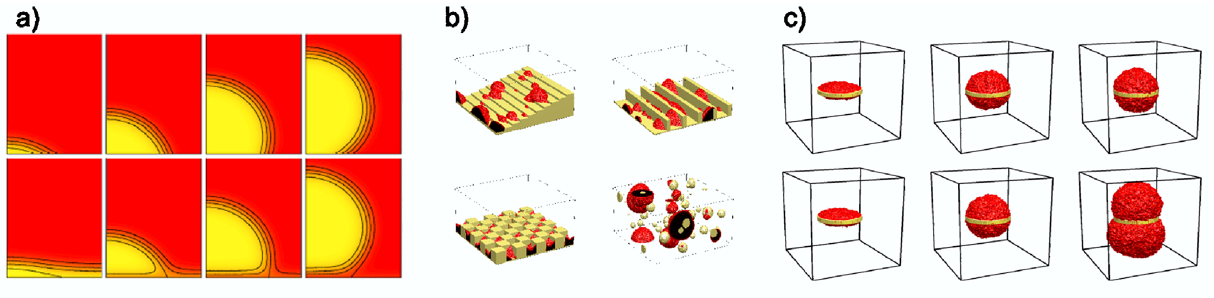

Special magnetic behaviour of (modified) Goethite dispersions

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Colloidal dispersions of boardlike alpha-FeOOH (Goethite) show very rich phase behaviour including nematic, smectic and columnar liquid crystals [1,2]. Here, we discuss these different phases and the role polydispersity plays in their appearance. We also address the peculiar behaviour of these particles and phases within an external magnetic field due to a small permanent moment along the long axis and an induced moment largest along the shortest axis of the Goethite particles. The balance between these two counteracting orientation mechanisms is shown to shift to higher magnetic fields if ions such as chromium are incorporated within the Goethite particles.

[1] B.J. Lemaire, P. Davidson et al. Phys. Rev. Lett. 88 (2002), 125507

[2] G.J. Vroege, D.M.E. Thies-Weesie, A.V. Petukhov, B.J. Lemaire, and P. Davidson, Adv. Mat. 18 (2006), 2565

T - 33

Random Organization: A nonequilibrium dynamical transition in periodically strained suspensions

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It is well known that when a fluid between concentric cylinders is strained (i.e. sheared) by boundary motion that is subsequently reversed, then all fluid elements return to their starting positions, provided the Reynolds Re number is small. We find that when a suspension of non-Brownian neutrally-buoyant particles is periodically strained at low Re, reversibility initially fails as a result of particle collisions. However, if the amplitude of the strain is below some critical threshold, the random displacements caused by particle collisions lead to a self-organized state in which the particles cease to collide after some time. The time scale for this self-organization exhibits a power-law divergence as the critical strain threshold is approached from above or below the threshold, suggesting that the transition is some kind of critical point. We introduce a simple model to describe this nonequilibrium phase transition. In the model, particles that collide under externally driven shear flow are given small random displacements to mimic the irreversible particle movements observed in experiment. The model exhibits two regimes: at low density, the random displacements lead to increased organization until a configuration develops where particles never collide and irreversible motion ceases. At high density, the collisions never cease. A sharp critical transition separates the two regimes. This simple model exhibits remarkable agreement with the experiments. More generally, the model and experiments reveal how driven dynamical systems can organize to find non-trivial absorbing states through purely random non-directed dynamics.

T - 34

Revealing the interplay of forces: dewetting fluids, adsorbing proteins and sticking geckos

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Intermolecular forces embrace all forms of matter and are also present in our every-day life as they e.g. determine the strength of a glue or the wetting properties of water on textiles. In my talk I will describe our way to access these forces by studying thin liquid films in the nanometer range [1]. The lessons learned can then be applied to more complex situations as, e.g., the adsorption of proteins to surfaces like dental implant materials [2] or the adhesion of geckos [3].

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CONFERENCE POSTERS

P - 1

Induce nematic phase in rigid rods driven by an elongational flow

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It is described the alignment in colloids of very long and thin rods induced by an elongational fluid by computing the self orientational structure factor [1]. The importance of this quantity is that it can be probed in a depolarized light scattering experiment. The incident polarization is assumed in the z-direction whereas the scattered in the XY plane. The structure factor is computed by using the solution of the stationary Smoluchowski equation neglecting hydrodynamic interactions. The torque involved is computed in absence of the external flow and using the Maier-Saupe potential, where the order parameter tensor is obtained by minimizing the free energy [2]. Results are presented, as function of the dimensionless rotational Peclet number and the scaled volume fraction, for nematics director perpendicular and parallel to the plane of the elongational flow. The results predict the values of the parameters in which the alignment is reached and these depend on the director's direction. One observation is that the fourth order parameter is also important in the description of the nematic-like phase.

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[2] M. Doi and S. F. Edwars, The Theory of Polymer Dynamics, Oxford Science Publications (1995).

P - 2

Structure of a Mixture of Colloidal Dumbbells and Spheres

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The static structure of a colloidal system consisting of dumbbells in a suspension of spherical particles, confined in a quasi-two-dimensional geometry, is measured by optical microscopy. Colloidal dumbbells are fabricated by inducing colloidal aggregation followed by sintering. The particles are confined between two parallel plates in order to form a quasi-two-dimensional system. Measurements of the correlation functions dumbbell-sphere, and sphere-sphere are presented for different sizes of particles.

P - 3

Binary crystals in strongly confined colloids described by a two-dimensional Yukawa interaction

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The zero-temperature phase diagram of binary mixtures of particles interacting via a screened Coulomb potential pair potential (Yukawa potential) is calculated as a function of composition and charge ratio. The potential energy obtained by a lattice summation is minimized among a variety of candidate two-dimensional crystals. A wealth of different stable crystal structures is identified including A_nB_m structures with $n = 1, 2, 3, 4$ and $m = 1, 2, 3, 4, 6$. [A (B) particles correspond to large (small) charge.] Their elementary cells consist of triangular, square or rhombic lattices of the A particles with a basis comprising various structures of A and B particles. These structures are detectable in experiments on confined mixtures of charged colloids.

P - 4

AC field-induced shape change of nematic liquid crystalline droplets

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We investigate the influence of AC fields on nematic liquid crystalline droplets coexisting with and immersed in a continuous isotropic phase of the same mesogenic liquid. Its dielectric constant and (small but non-vanishing) electric conductivity depend on both the phase and the orientation. These dependences can give rise to convective motion in the nematic phase (electro-hydrodynamic convection, EHC) or near the droplet surface (leaky dielectric model, LDM). Due to the extremely low surface tension of nematic-isotropic interface, viscous stresses easily can induce substantial deformations visible under the microscope.

We follow the influence of frequency and electric field strength on the deformation of the droplets for liquid crystals with positive and negative dielectric anisotropy (5CB and MBBA). In both cases we find a disk-like (oblate) deformation which shows a maximum when plotted as a function of frequency at constant applied field. Isotropic droplets in a nematic surrounding behave in a similar manner but show an elongation (prolate deformation). Depending on the initial size of the droplets, the interaction between neighboring droplets is either attractive or repulsive. Added tracer particles in the isotropic phase reveal a convective motion around the nematic droplets driving the deformation of the droplet. We interpret our findings in the frame work of the LDM and find good agreement.

Shear-induced structural changes in nanoparticle aggregates: a time-resolved x-ray microscopy study

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X-ray microscopy is an imaging technique which allows for a spatial resolution below 35 nm. Can it also be used to investigate shear-induced structural dynamics? When studying response to mechanical (shear) stimuli, the challenge lies in applying the stimuli with precision comparable to spatial resolution. We accomplished this by inserting a piezo actuator-driven shear cell into the focal plane of the x-ray microscope. We demonstrate the possibilities of this novel device by an investigation of shear-induced reorganization of 50 nm sized magnetite particles embedded in a polymer melt. As x-ray microscopy proves suitable for studying structural change, new prospects open up in physics at small length scales.

P - 6

Phase Field Crystal (PFC): continuum simulations on atomistic scales

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The phase field crystal (PFC) is a relatively new approach to extend classical phase field (PF) models for phase change problems to atomistic length scales. PFC was first pragmatically introduced by construction of a free energy, that is minimized by a periodically varying order parameter [1]. Thereby, the maxima of the order parameter represent the positions of single atoms in bulk material. In addition, regions of slowly varying order parameter are identified as unordered phases, that is liquid or gas. Because of the periodicity of the order parameter, elasticity, anisotropy and defects in the crystal are naturally included in the PFC model. The dynamics is still governed on a diffusive timescale, as in PF.

Recently, the PFC has been connected to classical density functional theory (cDFT) of freezing [2,3]. Thus, the order parameter of PFC can be directly identified with a density wave of the material. Additionally, the PFC has been theoretically connected to classical PF by averaging techniques. Here, the order parameter of classical PF represents the amplitude of the density wave of PFC. Thus, the PFC is an interesting approach in between pure microscopical modeling, e.g. cDFT, and modeling of phase changes in a continuum limit with PF.

The PFC model obtained from the variation of the free energy is a nonlinear partial differential equation of at least sixth order. We solve this by a new semi-implicit discretization with finite elements [3]. We show that even in the most simple PFC model the equilibrium shapes of two dimensional crystals are dependent on modeling parameters such as temperature. The shapes vary between circles and perfect hexagons.

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[3] R. Backofen, A. Rätz, and A. Voigt, *Phil. Mag. Lett.*, 87:11, 2007.

P - 7

Self-assembly driven pattern formation of dendron-like macromolecules on a structured surface.

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Dendron–like macromolecules have been observed to self–assemble into a broad variety of patterns on top of graphite surfaces. We have developed a theoretical model to understand the nature of this assembly and explored the phase behavior as a function of temperature and density. The interaction between the macromolecules is described by an interaction–site model, which largely simplifies the complexity and reduces the model to a few points representing both the aromatic rings and carbonated chains of the molecule. The attraction between chains of different molecules is accounted for by a short ranged potential (Lennard-Jones), whereas the strong repulsion of the aromatic rings is encoded in a hard-sphere interaction. Suitable order parameters are introduced to describe the ensuing ordered phases and corresponding patterns. The phase behavior is explored employing extensive Monte-Carlo simulations.

P - 8

Dumbbell diffusion in a spatially periodic potential

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We present a numerical investigation of the Brownian motion and diffusion of a dumbbell in a two-dimensional periodic potential. Its dynamics is described by a Langevin model including the hydrodynamic interaction. With increasing values of the amplitude of the potential we find along the modulated spatial directions a reduction of the diffusion constant and of the impact of the hydrodynamic interaction. For modulation amplitudes of the potential in the range of the thermal energy the dumbbell diffusion exhibits a pronounced local maximum at a wavelength of about 3/2 of the dumbbell extension. This is especially emphasized for stiff springs connecting the two beads.

P - 9

Colloidal plate dispersions out of equilibrium

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The last decade has witnessed the appearance of several experimentally convenient model systems of dispersions of colloidal plates, such as laponite and stabilized gibbsite particles. These complex fluids exhibit many interesting phenomena like gelation, glass transitions, as well as liquid crystal phase transitions. Meanwhile several theoretical studies have been devoted to *equilibrium* properties of the liquid crystal nature of platelet dispersions. This contribution reports on an investigation of *nonequilibrium* steady states of such systems by means of dynamic density functional theory.

P - 10

Charge induced conformational changes of dendrimers

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We study the effect of chargeable monomers on the conformation of dendrimers of low generation by computer simulations employing bare Coulomb interactions. The presence of the latter leads to an increase in size of the dendrimer due to a combined effect of electrostatic repulsion and the presence of counter-ions within the dendrimer, and also enhances a shell-like structure for the monomers of different generations. In the resulting structures the bond-length between monomers, especially near the center, will increase to facilitate a more effective usage of space in the outer-regions of the dendrimer.

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Driven colloidal particles as probes for stochastic thermodynamics

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The combination of colloidal particles and laser tweezers provides a powerful tool to experimentally investigate stochastic thermodynamics and fluctuation theorems. First we experimentally study the motion of a colloidal particle driven between two equilibrium states. While having an non-harmonic interaction potential, our data justifies the Jarzynski-Relation, however the observed distribution of work values W is non-Gaussian. In a second experiment we generate a nonequilibrium stationary state by means of rotating laser tweezers. Focusing on the entropy production we observe two regimes as a function of driving force. In both cases the fluctuation theorem holds for short trajectories, only when taking the entropy change of system and heat bath into account.

P - 12

Digital holography of dust clouds

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To describe the structural and dynamical properties of three dimensional particle arrangements an accurate knowledge of all particle positions and velocities at a given time is necessary. A measurement of the phase space evolution of such a system could be directly compared with results of analytic theory as well as Molecular-Dynamic or Monte-Carlo simulations. This would certainly help to gain insight into many interesting processes in strongly coupled media, e.g. diffusion, phase transitions, collective modes, etc. However, only a few diagnostics promise to fulfill the demanding requirements. Digital holography is one of them. This poster summarizes our recent progress to reconstruct the positions of particles with a few micrometer radius which are embedded in a plasma environment. The prospects and limitations of this method are discussed and compared to other diagnostic approaches (stereoscopy, color-gradient methods).

P - 13

Microscopic theory of liquid-vapour interface of inhomogeneous Lennard-Jones fluids

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A combined density functional theory and integral equations approach is used to study inhomogeneous Lennard-Jones fluids. It enables a microscopic description of the liquid-vapor interface through an explicit solution for the inhomogeneous two-body correlation functions. The method introduces a closure of reference hypernetted chain type to the inhomogeneous Ornstein-Zernike equation by employing a bridge functional of a suitably chosen hard-sphere reference system, which generalizes a conventional bridge function approach. For the liquid-vapor interface, we obtained the density profile and the surface tension, as well as the inhomogeneous two-body correlation functions. The theory can be extended to mixtures and colloidal systems.

P - 14

Sedimentation of an attractive colloidal gel: concentration and velocity profiles' evolution

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We used an original depolarized light scattering technique, resolved both in space and in time, in order to investigate the sedimentation and the internal dynamics of a gel formed by colloidal particles interacting via depletion forces. Besides the evolution of the total height of the sediment $h(t_w)$, we were able to measure the local and instantaneous volume fraction $\phi(z, t_w)$, the sedimentation velocity $v(z, t_w)$ and the dynamics structure factor $f_s(z, t_w, \tau)$. We can thus realize a "cartography" of these three quantities at different instants t_w after the gel formation and at all the heights z. From preliminary results the height of the gel $h(t_w)$ shows at first a quick linear decrease with a two-steps concentration profile followed by a slow exponential relax. The density profile after several days experiences a gradual increase by going towards the bottom of the system, instead of the plateau observed during the first days. Sedimentation velocity decreases in time according to an exponential law, with a relaxation time comparable to that of the regime of slow diminution of $h(t_w)$. At fixed t_w, internal dynamics does not change with z and seems scale with the strain of the systems induced by gravity. On the contrary, $v(z, t_w)$ increase linearly with z and seems to saturate in the neighbourhood of the upper meniscus. This behaviour could suggest that the friction against the cell walls plays an important role in the kinetics of sedimentation as discussed in the models presented.

P - 15

Wet granulates under shear

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Small amounts of a wetting liquid render sand a stiff and moldable material. Cohesion between wet grains is caused by the presence of capillary bridges formed at the points of contact. The finite strength of these liquid bonds is responsible for a transition from a quiscient to a fluidized state under applied shear stress. This fluidization transition is studied in MD-type simulation in a two dimensional assembly of discs under the action of a spatially heterogeneous external force. Capillary interaction is modeled as a short ranged and hysteretic attractive force between discs with soft core repulsion. Besides the fluidization threshold, we studied the spatial and temporal distribution of granular temperature, shear rate, stress, local packing fraction, and density of capillary bridges in both the fluidized and the quiscient state. Alternatively to shearing induced by external forces we applied Lees-Edwards boundary conditions. In both cases the local viscosity in the fluidized state is dominated by the local packing fraction and diverges upon approaching random close packing.

P - 16

Structure of extremely confined colloids: a study by integral equations and simulation

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We consider the model of a binary colloidal mixture confined in a slit pore that can accommodate only one big macroparticle in the direction normal to the walls. Structural quantities and the wall-macroparticle potential of mean force are studied in extreme conditions that combine the effect of strong confinement and short range attractions between the colloids. We compare results obtained by simulation and by a recently proposed integral equation method [1] based on bridge functions derived from Rosenfeld's hard sphere functional used in the reference hypernetted chain closure of the Ornstein-Zernike equations, the inhomogeneity being treated following the technique of Henderson, Abraham and Barker. Agreement between the two approaches validates the method. Various situations are presented that underline the competition between entropic and solvation forces. The effect on an external field will also be considered.

[1] A. Ayadim, J.G. Malherbe and S. Amokrane; J. Chem. Phys., 122, 234908, **2005**; S. Amokrane, A. Ayadim and J.G. Malherbe, J. Phys. Chem. C. 111, 15982, **2007**.

P - 17

Thermodynamics, structure and effective interactions in charge-stabilized colloidal suspensions

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We study the thermodynamics and structure of highly charged colloidal suspensions using a mean-field theory, integral equations theory and primitive model computer simulations. We suggest a simple way to include the macroion correlations into the mean-field theory as an extension of the so-called renormalized jellium model. The effective screening parameters extracted from our mean-field approach are then used in a one-component-model with macroions interacting via a Yukawa-like potential to predict macroion distributions. We find that inclusion of macroion correlations leads to a weaker screening and hence smaller effective macroion charge and lower osmotic pressure of the colloidal dispersion as compared to other mean-field models. This result is supported by comparison to primitive model simulations and experiments for charged macroions in the low-salt regime, where the macroion correlations are expected to be significant.

Enhancing effects of shear on crystall nucleation in colloidal suspensions

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Extensive two-dimensional Brownian Dynamic simulations are used to determine the effect of non-periodic shear in the crystal nucleation kinetics of charge stabilised (Yukawa repulsive) colloids, and attractive colloids (polymer-depletion driven colloids). Results show that in both systems small amounts of shear can speed-up the crystallisation process and even enhance the quality of the crystal. Insight about the crystal state enhancement (destruction) at low (high) shear rates is provided in terms of the dual nature of shear: shear tends to separate particles that form a nucleus, but at the same time induces an extra flux of matter that increases the frequency of collisions with the nucleus that speed up the process of aggregation. In addition to the analysis of the crystal nucleation phenomena, a characterisation of the transport properties and the steady state as a function of the shear is performed.

P - 19

From Soliton staircases to strain density waves: Monte Carlo Simulations of surface-induced deformation of soft colloidal crystals

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Two dimensional colloidal crystal interacting with an inverse power law potential was studied using Monte Carlo simulations [1,2]. Two structured walls, which are created by choosing two rows of particles fixed in the positions of the triangular lattice, provide the confinement to the system. By varying the distance between two walls, the deformation of the two dimensional colloid is induced and the typical soliton staircase can be observed [3]. The strain in the system was calculated and the standing strain wave superstructure was found in the different thicknesses of the strips. On the other hand, the melting of colloidal crystal was also studied.

[1] A. Ricci, P. Nielaba, S. Sengupta and K. Binder, Physical Review E 75, 011405 (2007).
[2] A. Ricci, P. Nielaba, S. Sengupta and K. Binder, Physical Review E 74, 010404(R) (2006).
[3] Y. H. Chui, S. Sengupta and K. Binder, submitted for publication.

P - 20

Gibbs ensemble simulations of discrete fluids

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We performed Gibbs Ensemble Monte Carlo simulations to investigate the liquid-vapor phase diagram of discrete potential fluids. Previous work has been reported, for instance, for square-well (SW) discrete fluids. In this work we study potentials with (i) a square-well plus a square-barrier (SWB) and, (ii) a square-well plus a square-barrier plus a square-well (SWBW), to model fluids that include a barrier after the primary minimum and fluids with a secondary minimum, respectively. Results are presented for the liquid-vapor phase diagrams and critical points, and for the pressure and chemical potential at coexistence. We find that the properties of these systems, especially the coexistence curves, are highly dependent on the strength of the barrier and the second well, even at weak couplings. Some of the trends that we observe here are similar to those observed in attractive Yukawa fluids.

P - 21

Effect of Interactions on Structural Transition in Bilayer Crystals

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Structural transitions in solid under confinement have been studied extensively through experiments and computer simulations on colloidal hard-sphere systems. A generic sequence for this transition : $n\triangle \rightarrow (n+1)\square \rightarrow (n+1)\triangle$ has been observed. However, the nature of such confinement induced structural transitions especially the effect of the interaction potential on such transitions has not been studied in detail. We attempt to do this by focussing on crystalline bilayer systems interacting with two widely known pair-interactions, namely the Lennard-Jones and Gaussian core potentials. Using zero temperature and finite temperature calculations we establish that this transition is generic, though the order depends crucially on the nature of the potential. For the Lennard-Jones system we obtain a first order transition whereas the purely repulsive and soft Gaussian core potential shows a continuous transition.

P - 22

Stabilizing a two-dimensional crystal by substrate potentials: pinning, depinning and the role of disorder

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Monte-Carlo data are presented of two-dimensional colloidal systems that are exposed to (i) a commensurate hexagonal substrate with filling factor $\eta = 1/9$, and (ii) a completely randomized substrate. When $\eta < 1$ such systems can form both a pinned and a floating solid phase. In the first case the colloidal crystal is registered to the periodicity of the substrate, thus adopting its perfect order, while in the second case, the floating solid, the order resembles that of a free crystal. Phase-diagrams are caluculated that show the transition lines of pinned → floating, floating → liquid, and pinned → liquid. Having studied how an ordered substrate stabilizes a 2D solid phase, we then ask the reverse question as to whether a disordered (glassy) substrate is capable of enforcing a glassy phase, thus destroying the order of a 2D solid. This question is discussed in the context of the peculiar pinned/floating scenario for systems with $\eta < 1$.

P - 23

Two-dimensional crystallization of magnetic dipoles

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We study the crystallisation process of a two dimensional system of superparamagnetic colloidal particles. By applying an external magnetic field perpendicular to the sample plane the repulsive dipole-dipole interaction between the particles and therefore the system temperature can be adjusted over a wide range. Video microscopy yields exact time dependent positions of several thousand particles on all relevant length- and timescales.

Using positional data we apply the local bond order parameter to distinguish particles in the crystalline form from those in the fluid. This allows us to identify crystalline regions. By tracking those areas over time we can observe the nucleation process and the growth of colloidal crystals in case of a temperature quench below the melting temperature.

P - 24

Optical Tweezers to measure the interaction between Poly(acrylic acid) Brushes.

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Optical Tweezers have been used for the evaluation of the interaction forces between poly (acrylic acid) brushes. The optical tweezers setup permit to access at forces in the range of 0 – 10 pN with a resolution of ± 0.3 pN . In this work we present evolution of the forces varying the ionic strength, the pH and the valence of the surrounding medium. The experimental data is fitted with a previously developed theoretical model which takes into account the entropic effect of the counterions. Excellent agreement between experimental data and the model was observed. By this way it's possible to estimate the brush height and the salt concentration inside of the brush which is higher than in the bulk for low salt concentrations.

P - 25

Rheology and particle tracking on soft colloidal suspensions with tunable glassiness

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We studied both the macro- and micro- rheology of soft thermosensitive microgel suspensions that can be tuned continuously and reversibly between the glassy state at low and the liquid state at high temperature. In the glassy state, the rheological properties (G', G", and J) of the suspensions depend strongly on their age [1]. They can be described quantitatively by the soft glassy rheology (SGR) model. The underlying mechanism for the aging is the increase of the structural relaxation time as the system ages. To test for micro-rheological properties we determined the mean square displacement (MSD) of probe particles, embedded in the system. The MSD values were obtained from particle tracking using a Confocal Scanning Laser Microscope. This technique provides not only the MSD values but also the displacement distributions and the time evolution of single particle displacements, which are indicative for heterogeneity of the suspension. In this paper we will discuss the non Gaussian properties of our suspension at different levels of glassines as well as the relation between these properties and the macro-rheology.

[1] E.H. Purnomo, D. van den Ende, J. Mellema, and F. Mugele, Phys. Rev. E. 76, 021404 (2007).

P - 26

A relationship of mean-field theory for a driven lattice gas to an exact equilibrium density functional

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We consider the totally asymmetric exclusion process (TASEP) of particles on a one-dimensional lattice that interact with site exclusion and are driven into one direction only. The mean-field approximation of the dynamical equation for the one-particle density of this model is shown to be equivalent to the exact Euler-Lagrange equations for the equilibrium density profiles of a binary mixture. In this mixture particles occupy one (two) lattice sites and correspond to resting (moving) particles in the TASEP. Despite the strict absence of bulk phase transitions in the equilibrium mixture, the influence of the density-dependent external potentials is shown to induce abrupt changes in the one-body density that are equivalent to the exact out-of-equilibrium phase transitions between steady states in the TASEP with open boundaries.

P - 27

Dynamics and local order in a 2D colloidal glass former

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Using video microscopy we study a two-dimensional binary mixture of superparamagnetic particles at a water-air interface. This provides time dependent particle coordinates of about 3000 particles on all relevant time- and length scales. The effective system temperature is controlled by tuning the interaction potential of the particles by an external magnetic field applied perpendicular to the interface. Typical features of a glass former are found. Increasing the magnetic field strength the system traverses from a fluid to a dynamically arrested state while staying amorphous. A comparison of mean square displacements with 'Mode Coupling Theory' of a hard disc glass former is presented. At low fields partial clustering of the small particles occurs in an equilibrium fluid phase. This sponge-like topology at low fields is accompanied by a characteristic small-wave vector peak in the small-small structure factor which is shown in a comparison of experiment, computer simulation and theory. Topological investigations using Euler characteristics also confirm this behavior. The local structure as obtained by pair correlation functions and bond order statistics is investigated as a function of system temperature and relative concentration. Although the system has no long range order and exhibits glassy dynamics, different types of stable crystallites coexist. The local order of the globally disordered structure is explained by a small set of specific crystal structures. The statistics of crystal unit cells show a continuous increase of local order with decreasing system temperature as well as a dependence on sample history and local composition.

P - 28

Charged Colloidal Rods: Pair interactions and excluded volume of finite length charged colloidal rods

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We present a theoretical investigation on the phase behaviour of charged colloidal rods suspended in electrolyte. Using a second-order virial expansion, we extend the previous work on charged rods. This work was initiated by Lars Onsager and deals with the limit in which the rod length is much larger than the Debye screening length. In the case of finite lengths, we calculate effective rod dimensions and investigate the angular dependence of the effective excluded volume. We make use of a continuum limit of the Yukawa segment model and expand the Yukawa (i.e. screened Coulomb) potential in spherical harmonics. This enables us to do fast calculations and easily sample the vast parameter space.

P - 29

Non-equilibrium response of colloidal particles in a microfluidic device

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We consider a dilute suspension of colloidal particles confined in a topographically structured microfluidic channel. When driven away from thermal equilibrium by time-dependent electrical fields, the average motion of the colloidal particles is opposite to the mean external force, i.e. the particles show negative mobility. The underlying physical mechanisms are illustrated, and theoretical predictions are compared with experimental results. The application of the effect for the separation of colloidal particles is discussed.

P - 30

Confocal microscopy of concentrated suspensions under confinement

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Concentrated colloidal suspensions under confinement appear in recently emerging technologies such as micro fluidic synthesis of anisotropic colloids and several Lab on a chip applications. Unwanted wall-particle interaction and channel clogging are the principle obstacles in development of such technologies. Despite the recent developments in control of flow and manipulation of colloids in micro fluidic devices; lack of control over structure formation under confinement in the vicinity of walls is the fundamental problem underlying mentioned obstacles. In this poster, we are representing a force sensor so called confinement apparatus integrated with Confocal Scanning Laser Microscopy (CSLM). Confinement apparatus is a double cantilever design with strain gauges for force measurements. Integration of confinement apparatus with Confocal Scanning Laser Microscopy allowed us to observe Quasi-Static dynamics of concentrated colloidal suspensions in real time and measure confining forces simultaneously. Quasi-Static dynamics of concentrated suspensions were studied by particle tracking (PT) and particle imaging velocimetry (PIV).In our experiments, we worked on 20 micron thick colloidal layers made of 1.2 micron diameter shell-core fluorescent colloidal particles prepared under gravity field indented with 1 mm glass ball.

P - 31

Binary Hard Sphere Crystal Structures Predicted Using Genetic Algorithms

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We study the close packed structures of binary hard spheres for various stoichiometries and small-to-large sphere diameter ratios using a genetic algorithm. Instead of relying on a set of pre-selected structures, the genetic algorithm is used to search the entire phase space of all possible structures with only the maximum number of elements in the unit cell restricted. In addition to predicting many of the known structures, such as NaCl and AlB_2, we find additional phase structures which may play a role in the phase diagrams of hard spheres with small-to-large sphere diameter ratios near 0.8.

P - 32

Binary Mixture of Eye Lens Proteins: a colloidal approach

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Mammals eye lens is a quite unique organ. It contains three families of soluble proteins: alpha, beta and gamma crystallin. In order to achieve the necessary refractive index the concentration in the lens is relatively high. When uncontrolled aggregation occurs the transparency of the lens is compromised. This mechanism is what causes the cataract disease, one of the leading cause of blindness. We numerically studied binary mixtures of alpha and gamma proteins developing an interaction model that could reproduce SANS and SAXS data. Gamma proteins are known to be attractive and to possess a liquid-liquid phase separation at low temperatures while alpha are purely repulsive. We show that when mixtures of these two proteins are considered an effective attraction between unlike species must be introduced to better reproduce the experimental results. We will show how this new attraction stabilizes the solutions and prevents the gamma crystallin from aggregation and that its intensity must be fixed in a very narrow window: if it is too strong the system becomes unstable again. The use of thermodynamic perturbation theory gives a first indication of the structure of the full phase diagram.
It is well established that the presence of Alpha crystallins in the eye lens prevents aggregation via different chaperon-like properties but this is the first time that one route to such activities is explained on a colloidal basis.

P - 33

Cluster-formation vs. lane-formation in two-dimensional square shoulder systems

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We predict minimum energy configurations of the two-dimensional square shoulder system for different values of corona width by employing search strategies based to genetic algorithms. In dependence of the pressure applied and of the corona width we obtain complete sequences of minimum energy configurations, consisting of a variety of non-trivial structures. The results provide a deeper understanding of the system's strategies to arrange particles in an energetically favourable fashion, a consequence of which are competing self-assembly scenarios of cluster-formation vs. lane-formation.

P - 34

Equilibrium structures of binary systems on a plane, investigated by genetic algorithms

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Genetic algorithms (GAs) are powerful tools, applied in many fields of physics as they offer an efficient strategy in high-dimensional optimisation problems. We have developed GA-techniques that allow us to study equilibrium crystal structures in an unbiased and parameter-free way. Recently we have refined our approach and extended it to binary mixtures of dipolar particles in a two-dimensional geometry, realisable in experiments via, e.g. magnetic colloids on a pendant water droplet and exposed to an external field or, equivalently, via polystyrene particles floating at an oil-water-interface. Several non-trivial and exotic structures are discovered and their dependence on concentration and size ratio of the particle species is discussed.

P - 35

Computer Simulations and Experiments on Colloidal Crystals: Elastic Constants, Effects of Boundaries and External Fields

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The phase diagram of a binary hard disk mixture (diameter ratio $\sigma_B/\sigma_A = 0.414$) in an external periodic potential is investigated by Monte Carlo simulations. The interaction with the substrate completely changes the miscibility of the binary mixture. In addition such a system exhibits a field induced ordering transition and a so called fissuring regime. We show that these phenomena are to be found even in purely repulsive systems as a 2D hard disk mixture [1]. Generic effects of confinement on crystalline order in 2D are studied [2] by Monte Carlo computer simulations of point particles interacting via a potential $\propto r^{-12}$. The state of the system (a strip of width D) depends very sensitively on the precise boundary conditions at the two confining walls. Commensurate, corrugated boundary conditions enhance both orientational order and positional order, so surface-induced order persists near the boundaries at temperatures where the system in the bulk is in its fluid state. In contrast smooth repulsive boundaries enhance only the orientational order and destroy positional (quasi-)long range order. The elastic properties of fcc crystals consisting of charge stabilized colloids are determined from real space imaging experiments using confocal microscopy [3]. We show that the Cauchy relation is not fulfilled and that only non-central many-body forces can account for the elastic properties.

[1] K. Franzrahe, P. Nielaba , Phys. Rev. E 76, 061503 (2007)
[2] A. Ricci, P. Nielaba, S. Sengupta, K. Binder,
Phys. Rev. E 74, 010404(R) (2006), ibid. E 75, 011405 (2007)
[3] D. Reinke, H. Stark, H.-H. von Grünberg, Andrew B. Schofield, G. Maret,
U. Gasser, Phys. Rev. Lett. 98, 038301 (2007)

P - 36

Mesoscale hydrodynamics approach to viscoelastic fluids

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Multi-particle collision (MPC) dynamics is a well-established, highly efficient particle-based hydrodynamics simulation technique for Newtonian fluids. The standard version of MPC does not conserve angular momentum. However, there are situations, where this leads to non-physical results. Therefore, we have developed a new method with angular momentum conservation.[1] We show that this method has to be employed, for example, to correctly describe circular Couette flow of multiphase fluids.[2]

Moreover, many complex fluids show viscoelastic behaviour. Therefore, an efficient MPC method for viscoelastic fluids is highly desirable. We present such an algorithm, that shows Maxwell fluid behaviour.

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Microrheology of dense colloidal suspensions from microscopic starting points

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We investigate the motion of a colloidal tracer, pulled through a colloidal suspension by an external force. For small forces, the difference between pulling with constant force or constant velocity, worked out in [1] for dilute suspensions, is studied for the case of dense suspensions. We use an approach based on the many-particle Smoluchowski equation and *mode-coupling* approximations, allowing us to include the possibility of a *glass transition*.

In the case of arbitrary force, the *nonlinear response* has to be considered. We start with the formally exact expressions for non-linear response and adopt the *intergration through transients* [2] method, developed for sheared suspensions, for our case. The key quantity of the approach is the time and external force dependent *density correlator* of the tracer. By means of mode-coupling approximations, a self-consistent equation is established for it, exhibiting many new properties (e.g. the correlator is, in general, complex) due to the *non-hermiticity* of the Smoluchowski operator in presence of the external force.

The mobility of the tracer strongly changes with applied force as surrounding particles are pushed aside for strong forces. The competition between internal diffusion and external drive leads to the *thinning* behaviour with increasing external force on the tracer. For a glassy suspension, our approach yields that the tracer can only move if the external force exceeds a threshold value. This *yielding* behaviour is in agreement with experiments [3] and simulations [4].

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DNA-driven assembly of micron sized colloids

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The highly specific nature of binding between base pairs in double stranded DNA offers many possibilities for the use of this biomolecule in technology for specific recognition on the molecular level. Here we present an experimental study in which we compare the self assembly of micron-sized PS beads bridged through hybridization of complemetary ssDNA strands (12bp) attached to variable-length dsDNA spacers that are grafted to the colloids. In all cases the same ssDNA pairs were used, however confocal microscopy revealed that the aggregation behavior is very different: ranging from finite-sized clusters to percolating systems.

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The effects of the ionic size asymmetry in the spherical electric double layer: a theoretical and simulational study

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We present the results of a Monte Carlo and integral equation study of the size-asymmetric spherical electric double layer (EDL). We used the primitive model of an electrolyte in order to mimic the 1:1 and 2:2 salts that surround a uniformly charged spherical colloid. Several interesting effects arise as consequences of the ionic size asymmetry, e.g. the occurrence of "overcharging" and of a characteristic non-monotonic behavior in the structural profiles (i.e. RDFs, potential, and integrated charge); besides we found that counterions do not always dominate the properties of the EDL. Some findings of the present work aware about the interpretation of electrophoretic mobility measurements using the standard electrokinetic theory (which is based in the classical Poisson-Boltzmann (PB) equation) beyond the validity region of the point-ions-based PB approach. Therefore, our primitive model treatment of the spherical EDL could serve as a starting point to improve such standard electrokinetic description.

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Crystal-like ordering of layered charged colloids in slit pores

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We consider a system consisting of two parallel walls filled with spherical charged colloids. The screening of the Coulomb potential of the macroions due to counterions and additional salt is taken into account via Yukawa theory. The applicability of this theory to real systems of charged silica spheres was proven by an earlier comparison of Monte Carlo results with colloidal probe AFM experiments [1]. Confined fluids typically exhibit a layering parallel to the walls, which was found for charged colloids as well [1,2]. Our current investigations focus on the in-plane structure in dense states using grand canonical Monte Carlo simulations. In particular, by computing bond angle order parameters and mean square displacements we search for evidence of crystallization in the layers. We discuss the dependence of the onset of crystallization on pore size and bulk density. Furthermore, we consider structural features such as the lattice type within the crystalline phases [3]. Finally, we discuss the influence of wall charges.

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Charged colloidal particles in a charged wedge: do they go in or out?

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The motion of highly charged colloidal particles which are confined between two a highly charged plates forming a wedge geometry is studied at low salt concentration by real-space experiments. It is found that a significant fraction of colloidal particles go inside the wedge. The experimental finding is discussed within linear screening theory and primitive model computer simulations.

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Scaling laws in the rheology of colloidal dispersions

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We have analyzed the shear flow behavior of dense colloidal dispersions close to the glass transition in the framework of a schematic version of mode-coupling theory (MCT). The schematic model contains the universal aspects of MCT [1] and was successfully applied to describe experimental data for the flow behavior and the linear viscoelasticity of thermosensitive core-shell dispersions [2].

We have derived a universal analytic expression which describes the flow curves quantitatively for small shear rates. This analytic expression provides a deeper understanding of the shapes of the flow curves. For instance, the scaling of the yield stress, the zero-shear limit of the shear stress, and its singular behavior at the glass transition point can easily be obtained by studying special asymptotic limits.

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Move it, shake it, anyway you want it - Combining Optical and Mechanincal Methods to Control Optical Tweezer Arrays

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We have constructed Optical Tweezers combining a Holographic Element and Mirror Galvanometers. Using the Holographic Element we can create arrays of large numbers of traps in three dimensions and update each trap at up to 5 Hz. Using the Galvanometric Mirrors we can translate the entire trap array in two dimensions over the field of view at frequencies of up to 1kHz. Combining the two techniques allows us to use the strong points of each without suffering from the weakness, i.e. the slow dynamics of the Holographic Manipulation and the lack of flexibility of the Galvanometers. We are using the set up to promote crystallisation in colloidal systems using a variety of different static and dynamic templates.

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Simulation Studies of the Transport Behavior of Colloids in Micro-Channels

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The transport behavior of a two-dimensional (2D) system of gravitationally driven colloidal particles is investigated by simulation of the overdamped Langevin equations neglecting hydrodynamic interactions. The $1/r^3$ dipolar particle interactions are given due to application of an external magnetic field perpendicular to the 2D sheet of superparamagnetic particles. For strong particle coupling a layered structure forms parallel to the confining walls. This arrangement of the particles is perturbed by diffusion, and directed motion is induced by gravity. Due to these combined influences a density gradient forms along the direction of motion of the particles. A reconfiguration of the ordered structure is observed leading to a reduction of the number of layers. The particles flow across the position of the layer reduction which itself remains relatively fixed in position. Both experiments and simulations show that the layer reduction occurs due to the density gradient along the channel. [1] Additionally, the influence of single and multiple line barriers perpendicular to the flow direction on the particle transport will be discussed.
Furthermore we will present simulation results for channel crossings of Y-shape where the mixing behavior of the particles in the outflow channel is analyzed. We find that the particle mixing occurs depending on the particle interaction strength which can be tuned by the external magnetic field.
Effects like particle blocking and formation of lanes are found for two different particle species which are driven in opposite directions within the microchannel.

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P - 45

Glass transition in colloidal hard spheres

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Using Molecular Dynamics simulations, we study suspensions of pure and polydisperse hard spheres at volume fractions along the metastable extension of the fluid branch. We calculate very accurately the equation of state and observe a sudden deviation from the fluid equation of state proposed by Speedy at a volume fraction of about 57.7±0.3. A closer study of this deviation (only possible for polydisperse spheres) seems to indicate a kink in the compressibility and a discontinuity in the second derivative of the pressure as a function of volume fraction. Ageing of the system has a strong effect on the precise location of the discontinuity.

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Critical Casimir forces as a tool in colloidal suspensions

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Recently we measured the critical Casimir force between a colloidal particle and a substrate in a binary liquid mixture of water and lutidine.[1] Depending on the preference of the opposing surfaces for either lutidine or water the force can be tailored to be attractive or repulsive. Its strength can be easily tuned via a variation in temperature. Applying the critical Casimir force to multi particle systems we can create colloidal monolayers or arrange colloids in a variety of patterns via a chemical treatment of the substrate.
[1] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich, C. Bechinger, Nature 451, 172 (2008).

P - 47

Dynamics in inhomogeneous liquids via the test particle limit.

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We show that one may view the self and distinct parts of the van Hove dynamic correlation function as the one-body density distributions of a binary mixture. These are taken to evolve in time according to dynamical density functional theory. For a test case of soft-core Brownian particles the theory yields results for the bulk van Hove function that agree quantitatively with those of our Brownian dynamics computer simulations. The free energy underlying the dynamics is found to be monotonically decreasing as a function of time. Using a related approach based on equilibrium density functional theory, we find that for hard spheres, at sufficiently high densities, the free energy exhibits a barrier as a function of the mean particle displacement. We interpret this barrier as the result of temporary caging of particles by their neighbours, shedding light on the nature of glass formation. For hard spheres confined by one wall or two parallel walls the barrier height oscillates in-phase with the local density, implying that the mobility is maximal between layers. Furthermore by considering a free energy landscape that varies with the direction of particle displacement we find that particles within layers are more likely to move in the directions parallel to the walls rather than perpendicular. These results should be observable in experiments of confined colloidal dispersions and in computer simulation.

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Shear induced aggregation of ‘wet’ particles floating at an air-liquid interface

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Granular materials may behave like solid, liquid or gas provided that energy is continuously injected to compensate for the dissipation due to inter-particle collisions and friction with the ambient fluid phase[1]. Here we present an experimental study of the dynamics of a 2D granulate of spherical particles floating at the interface of an aqueous liquid. The particles are driven by a shear flow of the liquid controlled by the rotation speed of the shear cell. The particles can be wetted by an oil phase giving rise to a hysteretic and short ranged capillary interaction[2]. The movement of particles under shear flow is captured by a high speed camera and the images captured are in turn subjected to image processing which enables tracing of individual particles. With this setup, the formation, growing and merging of clusters as well as its dependence on the driving shear force are studied and compared to numerical simulations.

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Effective interaction between star polymers under different solvent conditions

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We investigate the conformations of star polymers in solvents of different quality, especially for situations near the θ–point. We perform monomer resolved molecular dynamics simulations to derive the effective star-star interaction and its dependence on different solvent conditions. Additionally, we present a theoretical approach for the interaction and compare the results with corresponding simulation data.

Behavior of two-dimensional nematic colloidal crystals in the presence of an electric field

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The behavior of two-dimensional nematic colloidal crystals in the presence of an electric field will be presented. When colloidal particles are confined to a thin layer of a nematic liquid crystal, topological defects are formed, binding colloids together. I have used laser tweezers to assemble two-dimensional colloidal crystals. An electric field exerts torque on the molecules of the liquid crystal, causing reorientation. Consequently it has also an effect on the topological defects. With the application of an electric field perpendicular to the plane of the colloidal crystal we can change the distance between colloids. I have measured the relative changes in dimensions of colloidal crystals and characteristic times of this changes versus voltage, cell thickness, colloidal crystal size and temperature. When the light passes trough the colloidal crystal, it acts as a optical grid. With applying an electrical field we can change the lattice constant and consequently move the diffraction maxima.

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Crystallization kinetics in hard-sphere-like microgel colloids

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Colloidal systems display phase transition that are totally analogous to those observed in atomic systems. In particular, hard-sphere-like colloids form an ordered crystal phase upon increasing the particles volume fraction. Beyond the freezing line, the undercooling of the system acts as a driving force towards the formation of the solid phase. However, it is still a matter of theoretical and experimental investigations which path will the system actually follow in its journey towards the thermodynamically stable state, and which factors may influence it. Colloids are useful in order to investigate this issue, since they offer tunable interactions and time and length scales that are favourable for experimental investigation. Light scattering on polycrystalline colloidal samples provides the analogous of powder X-ray diffraction on atomic systems. With proper design of the experiment, it is possible to make time resolved measurements with satisfactory statistics starting from the very early stage of the crystallization process. This allows for monitoring the phase transition from the metastable fluid, to the onset of nucleation and growth of the crystallites, up to the later stage of ripening of the polycrystalline material. Experiments of this kind have profitably addressed some important issues concerning the crystallization kinetics in hard-sphere systems. Among these are the subtle effects of particle size polydispersity, and the qualitative changes that occur upon increasing the particle volume fraction, from low undercooling in the coexistence region, up to the approaching of the glass transition, where the driving force for crystallization is increasingly competing with dynamical arrest. These aspects will be reviewed while presenting recent results obtained in our lab with polystyrene microgel particles in an organic solvent, a system that has proved to display hard-sphere-like behaviour.

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String Phase in Electrorheological Complex Plasmas

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The so-called electrorheological (ER) fluids are the fluids where the interparticle interaction (and hence the rheology) is determined by external electric fields: At low fields they may be “normal” fluids, but above a critical field, at low shear stresses ER fluids behave like solids, and at stresses greater than a yield stress they flow with enhanced viscosity. ER liquids have significant potential for industrial applications – they can be used in, e.g., hydraulic valves, display production, photonics. Also, ER fluids have a remarkably diversified phase diagram that includes a number of (second-order) structural phase transitions.

We showed that interactions in complex plasmas induced by AC electric fields are very similar to those in conventional ER fluids. Complex plasmas can be carefully investigated at the most fundamental kinetic level. Therefore, the whole knowledge learned with ER complex plasmas can be directly applied to describe kinetics of conventional fluids. We found that when the amplitude of the ac field exceeds a threshold, a fluid complex plasma undergoes novel type of a phase transition, between an isotropic and a string phase.

Using the PK 3+ setup onboard ISS, we studied behavior of complex plasmas with an external AC electric field. The experiments confirmed the theory: At low fields the microparticles form isotropic gaseous-like phase, whereas above a certain threshold an ordering of particles along the field emerges. At sufficiently large fields the string fluid can be observed by naked eye. The magnitude of the critical field for the transition is in good agreement with the theoretical prediction. Also, numerical MD simulations were carried out, showing full agreement with the theory as well as experiments.

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Phase transitions in a quasi-two-dimensional Ising-model

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Inspired by the question, how hard spheres with parallel dipole moments in a gravitational potential acquit themselves, we study a more simple model to gain basic understanding. For this purpose an anisotropic Ising-model in three dimensions and in a gravitational potential was analytically analysed and simulated with the Monte-Carlo-method. The system containing a fixed number of hard particles, which carry a spin, is placed on a 3d lattice. The model is quasi two dimensional due to a surface at z=0 and due to the gravitation along the z-axis. In x/y-direction we use periodical boundary conditions. According to the dipole-dipole interaction, the applied nearest neighbour interaction is repulsive in x/y-direction and attractive in z-direction. The structures, which are formed in equilibrium, are examined for different particle densities, temperatures and coupling constants. In particular, we observe a non-trivial growth of towers of particles for high interaction strengths.

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Field–controlled layer formation in dipolar nanofilms

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Using molecular dynamic we investigate the equilibrium behavior of a dipolar model fluid confined between two plane parallel walls, focusing on the influence of an additional homogeneous external electric or magnetic field. Structural properties are examined for field directions parallel and perpendicular with respect to the walls. Confinement alone leads already to a preferred in–plane orientation of the dipole moments [1]. We demonstrate that external fields strongly influence and, in some cases, even change the structure in the system.

An important difference between the two field directions is that a perpendicular field gives a new preferential direction which competes with the in–plane orientation observed without field. As a consequence very large field strength are required to reach similar polarization values as with parallel field. Moreover a field perpendicular to the walls increases the occurrence of side–by–side alignment and therefore the overall repulsion. As a consequence the system develops more layers than without a field. The opposite effect can be generated by a parallel field which allows more energetically favorable head–to–tail configurations. Hence the particles can arrange in fewer layers than without a field [2].

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[2] J. Jordanovic and S. H. L. Klapp, in preparation.

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Depletion induced phase separation in suspensions of rod-like particles

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When non-adsorbing polymers are added to an isotropic suspension of rod-like colloids, the colloids effectively attract each other via depletion forces. We performed Monte Carlo simulations to study the phase diagram of such rod-polymer mixture. The colloidal rods were modeled as hard spherocylinders; the polymers were described as spheres of the same diameter as the rods. The polymers may overlap with no energy cost, while the overlap of polymers and rods is forbidden.

Large amounts of depletant cause phase separation of the mixture. We estimated the phase boundaries of isotropic-isotropic coexistence both, in the bulk and in confinement. To determine the phase boundaries we applied the grand canonical ensemble using successive umbrella sampling [J. Chem. Phys. 120, 10925 (2004)], and we performed a finite size scaling analysis to estimate the location of the critical point.

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Measuring Complex Flow Profiles in Systems with Shear Induced Phase Transitions by Super-Heterodyne Velocimetry

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Condensed matter put to extreme mechanical impact may react by crack formation, creep flow or even (partial) melting behaviour. Soft matter model systems may help in elucidating such phenomena due to both their softness, implying significant mechanical response even for small loads and their enlarged length and time scales, facilitating convenient optical access. Colloidal crystals in particular may display shear induced straining, local or global shear melting or shear induced crystallization, if subjected to shearing fields. Structural evolution may be monitored in detail using either video microscopy or time resolved static light scattering. We here show that incoherent scattering contributions (dominant at low scattering angles or selectively detected in VH geometry) can be exploited to provide the complementary information on the complex flow behaviour, without interference with the structural distribution. Super heterodyning in addition renders the data of interest free of homodyne contributions and low frequency noise. The combination of coherent and incoherent scattering experiments therefore may help in clarifying the coupling between structure and motion under shear. We exemplify our method studying an aqueous charged sphere suspension driven under the influence of different fields.

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Ordered equilibrium structures in layered systems

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We consider soft particles that interact via Gaussian pair potentials and investigate systematically ordered equilibrium structures that these particles form in a volume confined by two parallel horizonal walls which are separated by a distance D. Using search strategies that are based on ideas of genetic algorithms we identify the energetically most favourable particles arrangements as we vary the distance D and the number-density ϱ: these configurations are characterized by the number of layers that the system forms between the planes and the ordered equilibrium structures within each of the layers. A detailed phase diagram of the system is provided which allows the location of the transition lines between the emerging structures and the number of layers that the system forms.

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Forces of interaction between DNA – grafted colloids : An Optical tweezers measurement

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Optical tweezers are employed to measure the forces of interaction within a single pair of DNA-grafted colloids in dependence of the molecular weight of the DNA-chains (250 basepairs (bp), 500 bp, 750 bp, 1000 bp), the grafting density and the concentration and valence (mono-, di-, trivalent) of the surrounding ionic medium. The resulting forces are short-range and set in as the surface-to-surface distance between the colloidal cores reaches the value of the brush height. The measured force-distance relation is analyzed by means of a theoretical treatment that quantitatively describes the effects of compression of the chains on the surface of the opposite-lying colloid. Quantitative agreement with the experiment is obtained for all parameter combinations. Further experiments are carried out to measure under similar conditions the interaction between one DNA-grafted and one blank colloid. The results are discussed with respect to the different brush regimes.

K. Kegler, M. Salomo and F. Kremer, Phys. Rev. Lett. 98, 058304 (2007).
K. Kegler, M. Konieczny, G. Dominguez-Espinosa, C. Gutsche, M. Salomo, F. Kremer, and C.N. Likos, submitted to PRL

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Colloids in external electrical fields investigated by optical tweezers and ionic currents

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The charge of colloidal particles and macromolecules is of major importance for their interactions in aqueous solutions. Here we discuss experiments using optical tweezers and ionic current detection to study the characteristics of single colloids in electrolytes.

The motion of colloids in alternating electrical fields was studied by the application of optical tweezers and high-speed video detection [1]. Based on a newly developed fluidic cell, electrophoretic measurements [1] were carried out for Polystyrene colloids. The mobility as well as the zeta potential are examined for electrolytes of varying concentration and valence. Our experiments shed light on the interaction of electrophoresis and electroosmosis and account for the phase shift between the electric field and the colloidal response. Electrophoretic measurements were done in multivalent electrolytes verifying the reverse of the colloidal motion due to an excess of counter-ions also known as charge inversion.

Finally, we present first results for colloids driven through a glass capillary, very similar to the well known principle of Coulter counters. The passage of a single colloid is monitored by the brief blockage of the ionic conductance and an incorporated video detection system [2,3]. We deduce the charge of the colloid with experiments in various salt concentrations and compare the results with numerical models. We will also discuss the possibility to detect the grafting density of polymers on a single colloid.

1. Otto et. al., “Optical tweezers with 2.5 kHz bandwidth video detection for single colloid electrophoresis”, Review of Scientific Instruments, under review (2007)
2. Keyser et al., “Optical tweezers for force measurements on DNA in nanopores”, Review of Scientific Instruments 77, 105105 (2006)
3. Keyser et al., “Direct force measurements on DNA in a nanopore”, Nature Physics 2, 473 (2006)

P - 60

Fluctuation dissipation relations in stationary states of interacting Brownian particles under shear

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We study fluctuation dissipation relations in stationary states of interacting Brownian particles under shear theoretically. In computer simulation studies of glassy states, Berthier and Barrat [1] found the Fluctuation Dissipation Theorem (FDT) violated for particle motion in the vorticity direction, viz. perpendicular to the shear plane at long times,

$$\chi_f(t) = \begin{cases} \frac{-1}{k_B T}\,\frac{d}{dt}\,C_f(t) & \text{short times,} \\ \frac{-1}{k_B T_{\text{eff}}}\,\frac{d}{dt}\,C_f(t) & \text{long times.} \end{cases}$$

We investigate the phenomenon of an effective temperature T_{eff} via the recently developed mode coupling approach for sheared colloidal dispersions [2], starting from the Smoluchowski equation of the N-Brownian particle distribution function. The microscopic FDT relation [3] in non equilibrium is our exact starting point, which we analyze with mode coupling approximations. It is shown that our calculations are consistent with the findings in [1]. Furthermore we determine the value of T_{eff} for coherent density fluctuations in a full microscopic calculation.

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Colloidal potentials and near wall dynamics

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Averaged diffusivities of spherical colloids in solutions of rod–like particles, i. e. fd–virus, were measured with EWDLS and TIRM. While the experimentally observed near wall dynamics of the spheres in the absence of fd are well described by standard hydrodynamic theories, there are significant deviations at finite fd–concentrations. Both experimental methods yield data which are significantly smaller than the theoretical predictions.

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Viscoelasticity, Structure and Internal Dynamics of High Volume Fraction Colloidal Gels

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The experimental system investigated is mixtures of PMMA colloidal spheres and linear Polystyrene chains dispersed in cis-decalin. The polymer-colloid size ratio is such that short range attractions are induced between the colloids. The colloid volume fraction is kept constant at about 0.4, while the polymer concentration is increased gradually starting from the pure colloidal dispersion.

Samples along the constant volume fraction line have been investigated by Rheology, Dynamic and Static Light Scattering (DLS, SLS). Rheological measurements in the linear regime evidence a transition from fluid-like to solid-like response with increasing polymer concentration. Such a transition corresponds to the ergodic-non ergodic transition observed in 3D-DLS measurements of the same samples. In addition, formation of large scale network structures is confirmed by SLS. By further increasing polymer concentration in the solid, gel phase, the elastic modulus of the gel increases linearly. An increasingly pronounced solid-like behavior corresponds to slowing down of the collective dynamics, as obtained from DLS measurements.

Static light scattering measurements in the gel phase, together with confocal microscopy measurements, show important changes in the gel structure as soon as the polymer overlap concentration c* is exceeded. In particular, the degree of heterogeneity of the gels is found to decrease with increasing c* as well as the average number of neighbours per colloidal particle. In addition to the experimental results, we present a comparison between linear viscoelasticity data and theoretical predictions of a recently proposed MCT-based schematic model describing the rheological properties of colloidal gels and glasses [1].

[1] M. Fuchs and M. E. Cates, Phys. Rev. Lett. 89, 248304 (2002).

Structure and energetics of point defects in two-dimensional colloidal crystals

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We study the structure and the interaction of interstitials in two dimensional crystals. We compare the displacement field of these defects with elasticity theory. As a second part we study the interaction between these defects. Monte Carlo simulations showed that interstitials attract each other and form stable clusters. We show that the interaction between interstitials does not depend on the distance of the defects only, but also strongly depends on the symmetry of the defects and their orientation with respect to the underlying lattice. While the displacement fields of interstitials from the simulations are in very good agreement with the predictions from elasticity theory, the interaction between the defects is not predicted accurately by elasticity theory.

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Capillary interaction between ellipsoidal colloids at a fluid interface

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Partially wetting ellipsoidal colloids trapped at a fluid interface lead to considerable deformations of the equilibrium meniscus around them if the contact angle is different from 90^o. Recently, the meniscus profile and the resulting anisotropic capillary interactions have been investigated experimentally in the case of μm-sized ellipsoids at water-oil and water-air interfaces, respectively [1,2]. The results can qualitatively be explained by a quadrupolar meniscus profile caused by the particle's anisotropy which, however, appears to be considerably deformed for stretched ellipsoids. A thorough theoretical investigation of these phenomena is, however, missing so far.

The calculation of the exact meniscus shape around an ellipsoidal particle is a difficult numerical problem which requires the solution of a nonlinear partial differential equation together with Young's condition at the three phase contact line whose position on the colloid surface, however, is not *a priori* known. In a perturbative approach we derive a quadratic free energy functional of the interface and the colloids trapped at it. Minimizing the free energy allows for an efficient computation of both the meniscus profile and the capillary interaction in terms of an expansion into *elliptic* multipole moments. We discuss the shape of the equilibrium meniscus deformations and the resulting orientation dependent capillary forces in detail. As a further application, the configurations of minimal contact energy between two ellipsoids are determined which may have important influence on the experimentally observed formation of complex chain- or raftlike structures at the interface.

[1] J. C. Loudet, A. M. Alsayed, J. Zhang, and A. G. Yodh, Phys. Rev. Lett. **94**, 018301 (2005)
[2] J. C. Loudet, A. G. Yodh, and B. Pouligny, Phys. Rev. Lett. **97**, 018304 (2006)

Realizing Colloidal Artificial Ice on Arrays of Optical Traps

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We demonstrate how a colloidal version of artificial ice can be realized on optical trap lattices. Using numerical simulations, we show that this system obeys the ice rules and that for strong colloid-colloid interactions, an ordered ground state appears. We show that the ice-rule ordering can occur for systems with as few as 24 traps and that the ordering transition can be observed at constant temperature by varying the barrier strength of the traps.

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Evidence for re-entrant melting in star-like micellar solutions: a rheological and light scattering investigation

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We determined the rheological properties of aqueous solutions of star-like PEP-PEO block copolymer micelles by steady and oscillatory shear. A wide range of concentrations spanning from the very dilute to the highly concentrated regime was investigated ($0.17\Phi^* \leq \Phi \leq 5.5\Phi^*$). The structure of the individual micelle in terms of aggregation number, $f=78\pm5$ was characterized in dilute solution by small angle neutron scattering(SANS). Four different regimes in the concentration dependence of the zero shear viscosity η are experimentally observed. In dilute solution the intrinsic viscosity $[\eta]$ reflects the colloidal nature of the star-like micelles. With increasing concentration η_0 strongly increases, but contrary to star polymers and star-like micelles with higher functionality, no divergence of η_0 at Phi*is observed. Only at much higher concentrations, $\Phi \approx 2.8\Phi^*$, the zero shear viscosity η_0 finally diverges and solid like behavior is found, but only in an extremely small range of concentrations ($2.8\Phi^* \leq \Phi \leq 2.9\Phi^*$). Upon further increase of concentration the solutions melt again to a viscoelastic fluid (re-entrant melting) with a continuous decrease of η_0 up to $\Phi=5.5\Phi^*$, the maximum concentration under investigation. Similar trends are observed for results obtained from Light Scattering experiments. This is an experimental evidence of a re-entrant melting transition in the case of star-like objects, theoretically predicted for regular star polymers (ultra-soft colloids), but expected at lower functionalities.

[1] M.Laurati, J.Stellbrink, R.Lund, L.Willner, D.Richter and E.Zaccarelli Phys. Rev. Letters 94, 195504(2005)

[2] R.Lund, L.Willner, J.Stellbrink, and D.Richter Phys. Rev. Letters 96, 068302 (2006)

[3] M.Laurati, J.Stellbrink, R.Lund, L.Willner, D.Richter Phys. Rev E. 76, 041503 (2007)

[4] B.Lonetti, J.Stellbrink, L.Willner, D.Richter submitted to Macromolecules

PB-PEO wormlike micelles under oscillatory shear as probed by time-resolved SANS

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Worm-like micelles (WM) are known to undergo an isotropic (I) to nematic (N) phase transition upon concentration [1]. A complete microscopic description of their dynamical properties is still missing. We aim to gain this understanding by studying a versatile system of WM formed by a symmetric Poly(butadiene)-poly(ethylene oxide) (PB-PEO) in water solution by combining three different techniques: A novel time-resolved SANS measurement with rheology and high-speed confocal microscopy. PB-PEO micelles present the advantage, with respect to the more commonly studied surfactant WM, that they can be directly observed with fluorescence microscopy. Besides, changing the quality of the solvent allows playing on the micellar exchange kinetics (characteristic breaking time). The effect of the solvent composition on their equilibrium properties is investigated through SANS and fluorescence microscopy. We observe that the addition of DMF to aqueous solutions causes the cross-section diameter to diminish and eventually the transition from worm-like to ellipsoidal and spherical micelles. We are presently studying PB-PEO worm-like micelles in water in the vicinity of the I-N transition subjected to an oscillatory shear field. In order to sample the (non-)linear response of the worm Kuhn-segments during the oscillation we used time resolved SANS in the "stroboscopic" mode which provides a time-resolution of up to $\delta t = 5$ ms for periodic external fields. The thus obtained time-dependent alignment of the worm Kuhn-segments can be directly related to Fourier Transform Rheology data on the same system.

[1] You-Yeon Won, H. Ted Davis, Frank S. Bates Science 283 (1999) 960-963

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Correlations between phase behaviour and properties in charged colloidal mixtures

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Charged colloidal spheres in deionized aqueous suspension show a fluid-crystalline phase transition for sufficiently large and long-ranged potentials. For single component systems body centred cubic and face centred cubic structures have been observed by static light scattering. Microscopy revealed a polycrystalline morphology and torsional resonance spectroscopy showed that the elastic constants of the colloidal crystals are on the order of a few Pa. We here investigate binary mixtures of charged colloidal polystyrene spheres in deionized aqueous suspension whose colloidal components differ in size and charge. We observe a rich phase behaviour as a function of size and charge ratio including azeotropes of both kinds, indifferent spindle type phase diagrams and eutectics [1]. The contribution reviews the phase behaviour and the corresponding colloidal solid properties.

[1] N.Lorenz, J.Liu, T. Palberg: Phase behaviour of binary mixtures of colloidal charged spheres, Colloids Surf. A (in press 2007)

Colloidal hard dumbbells with and without gravity

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Using free energy calculations in Monte Carlo simulations we study the stability of orientationally disordered crystal phases in a suspensions of colloidal hard dumbbells. For dumbbell bond length $L/\sigma < 0.4$ with L the separation of the two spheres of the dumbbell and σ the diameter of the spheres, we determine the difference in Helmholtz free energy of a plastic crystal with a hexagonal-close-packed (hcp) and a face-centered-cubic (fcc) structure using thermodynamic integration and the lattice-switch Monte Carlo method. We find that the plastic crystal with the hcp structure is more stable than the one with the fcc structure for a large part of the stable plastic crystal regime. In addition, we study the stability of an orientationally disordered aperiodic crystal structure in which the spheres of the dumbbells are on an fcc lattice, and the dumbbells are formed by taking random pairs of neighboring spheres. Using free energy calculations, we determine the fluid-aperiodic crystal and periodic-aperiodic crystal coexistence regions for $L/\sigma > 0.9$. In addition, we perform grand canonical Monte Carlo simulations to study the effect of gravity on the hard dumbbell crystal structures. Surprisingly, the aperiodic crystal also forms in gravity, despite the bottom wall.

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Multiple glass transitions in star polymer mixtures

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We examine the vitrification and melting of asymmetric star polymer mixtures by combining rheological measurements with mode coupling theory and numerical simulations. In particular, we fix the concentration of the big stars just above their glass transition and vary concentration and size of the small star additives. In the plane spanned by size ratio and concentration of additives, we identify an "ergodic lake" surrounded by multiple glassy states characterized by different dynamic properties. At low concentration of additives, we find a single glass, where the small component is fluid in the glassy matrix of the big one, and a double glass, in which both components are vitrified, depending on the size ratio[1]. Addition of small star polymers leads to a melting of both glasses, and the melting curve has a non-monotonic dependence on the star-star size ratio. Upon further increase of the additive concentration, we find a re-vitrification into different glassy states, accompanied by interesting anomalous dynamics. Moreover, a novel "asymmetric glass", unique with respect to previously investigated systems, is found in the region of intermediate size disparity and high concentration of the small stars. These investigations open new ways for externally steering the rheological behaviour of soft matter systems.

[1] E. Zaccarelli *et al.*, Phys. Rev. Lett. **95**, 268301 (2005).

Long-time self-diffusion of charge-stabilized colloids and macromolecules

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The long-time self-diffusion coefficient, D^L, of charged colloids at non-zero concentration has been calculated via a consistent statistical mechanical theory which includes the hydrodynamic interactions (HI) between all particles, colloids and electrolyte ions, on the far-field level. The diffusion coefficient is found by calculating the friction acting on a single tracer colloid. This friction has several contributions: a colloidal contribution and the so-called electrolyte friction, which results from the non-instantaneous relaxation of the ionic atmosphere surrounding each colloid. The electrolyte friction is found to be negligible for large colloids, but may contribute significantly to the friction experienced by very small colloids, such as proteins, polymers and bio-molecules.

When the salt concentration is low, the charged colloids interact over a very large range so that the mean separation between the colloids scales as $\phi^{-1/3}$, where ϕ is the colloidal volume fraction. This scaling corresponds to a correlation hole around each colloid, which in turn leads to the domination of far-field HI. We find that this suppression of near-field HI causes an unexpected hydrodynamic enhancement of D^L, which manifests itself in a non-monotonic concentration dependence of D^L, as seen in recent experiments on DNA fragments. Furthermore, even though the renormalized effective charge also shows a similar non-monotonic concentration dependence in low salt suspensions, we show that the non-monotonicity of D^L is of purely hydrodynamic origin.

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Alternative Description of Dynamic Arrest in Colloid-Polymer Mixtures

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The reentrant glass transition involving "repulsive" and "attractive" glasses has been experimentally observed in dispersions of hard-sphere–like colloids with depletion interactions produced by the addition of non-adsorbing polymer [K. N. Pham et al., Science v. 296, p. 104 (2002)]. The prevailing belief is that a colloid-polymer mixture can be treated as an effective one-component fluid (the colloid) with polymer-mediated depletion forces described by effective "Asakura-Oosawa" interactions. This view, together with conventional mode coupling theory of dynamic arrest in mono-component systems, provides the conventional description of this experimentally-observed transition, since this reentrant scenario was first predicted by MCT, and since no alternative theory for these phenomena is available. This model, however, cannot explain important experimentally observed features, such as the detailed shape and location of the glass transition line. Although one obvious alternative view is to consider these systems as genuine highly size-asymmetric binary colloidal mixtures, no progress in this direction has been reported. Here we demonstrate that treating the colloid-polymer mixture within such perspective is indeed possible, and provides an adequate description of the dynamic arrest in these systems. Based on the recently-developed multi-component self-consistent generalized Langevin equation (SCGLE) theory of dynamic arrest, we find that, contrary to the common view, the dynamics of the polymer is as relevant as the dynamics of the colloidal species, and is directly responsible for the reentrant phenomenon in systems with depletion interactions. The remarkably precise agreement with the experimental glass transition line of a colloid polymer mixture seems to confirm this unexpected but conceptually simpler scenario.

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Electrophoretic deposition of metallic nanoparticles generated by femtosecond laser ablation in liquid media

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Femtosecond laser ablation in liquids is a technique which provides nanoparticles from a large variety of materials, dispersed in transparent liquids. Stable colloids can be fabricated for the study of their properties, free of impurities or additives. For our investigations on electrophoretic deposition of metallic nanoparticles on implants and electrodes for neural stimulation, we have generated from gold, silver and platinum-iridium alloy, nanoparticles in deionised water and acetone. Electric charging of the particles, induced during laser ablation, was studied by electrophoretic methods and particle visualisation using Rayleigh scattering. One-to-one nanoparticle tracking analysis, provided velocity distributions which were compared with electrophoretic mobilities measured by Laser Doppler Electrophoresis. Safe and effective nano-coating of conducting materials can be achieved by well-controlled electrophoretic deposition of the charged colloidal nanoparticles. Using an electrode as substrate, we have evaluated the influence of the voltage applied and deposition time on the resulting coating quality. Appropriate manipulation of the size, material, texture or depth of the nanoparticulate coating determines the future properties at the treated surface. At the example of neural electrodes, this method shows a great potential to improve biocompatibility, proliferative or antiproliferative effects, mechanical resistance and conductivity.

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Density functional theory for two-component mixtures of super-paramagnetic colloids

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The density functional theory of freezing is used to study the phase diagram of binary mixtures of super-paramagnetic colloidal particles in two dimensions. The particles interact via a purely repulsive potential which scales as inverse cube of inter-particle separations and are additionally exposed to an external magnetic field. The pair correlation functions needed as input information in density functional theory are calculated by hypernetted chain integral equation theory. A variety of different crystalline structures are found to stabilize relative to each other as a function of composition and the ratio of magnetic susceptibilities of the particles of the two components.

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Short-time Transport Properties in Colloidal Suspensions by Stokesian Dynamics Simulations

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This work includes the first comprehensive computer simulation study of short-time diffusion and rheological properties in concentrated suspensions of charge-stabilized and neutral colloidal particles. The particles in many of these systems are subject to significant many-body hydrodynamic interactions. A recently developed accelerated Stokesian Dynamics simulation (ASD) method is used to calculate a broad spectrum of transport properties, including hydrodynamic functions, wave-number-dependent collective diffusion coefficients, self-diffusion and sedimentation coefficients, and high-frequency-limiting viscosities. The dynamic properties are discussed in dependence on the particle concentration and salt content. Our ASD simulation results are compared with existing theoretical predictions, notably those of the renormalized density fluctuations expansion method of Beenakker and Mazur, and earlier simulation data on hard spheres. The application range, and the accuracy of various theoretical expressions for short-time properties, are explored through comparison with the simulation data. We analyze in particular the validity of generalized Stokes-Einstein relations relating short-time diffusion properties to the viscosity, and we point to the distinctly different behaviour of de-ionized charge-stabilized systems in comparison to hard spheres.

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The role of the capillary waves fluctuations in the interaction between ellipsoidal colloids trapped at fluid interfaces

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Knowledge of the effective interaction between nanocolloids at the interface of two fluids is one of the key parameters in the fabrication of ordered structures from such systems. This interaction involves a long-ranged part caused by capillary wave fluctuations [1]. Due to the restrictions which are imposed on the capillary waves by the colloids, the interaction is of Casimir type exhibiting longer-ranged power law decay in the inverse colloid distance. In the current work, the anisotropic Casimir interaction between two ellipsoidal colloids at the interface has been evaluated. This interaction might be of importance for ordering phenomena of nanoparticles, similar to the ordering which has been observed for microellipsoids [2].

[1] H. Lehle, M. Oettel, and S. Dietrich, Eur. Phys. Lett. 75, 174 (2006)
[2] J. C. Loudet, A. M. Alsayed, J. Zhang, and A. G. Yodh, Phys. Rev.Lett. 94 018301 (2005)

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Phase behaviour in mixtures of ultrasoft particles

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We investigate the phase behaviour of mixtures consisting of two ultrasoft species labelled A and B, using liquid state and classical density functional theories. We use the generalized exponential model ($\Phi(r) \sim exp[-(r/\sigma)^m]$) for both A-A ($m = 2$) and B-B ($m = 4$) interaction potentials. The two potentials belong to different classes of ultrasoft potentials that display dramatically different phase behaviour in the pure case: in pure A systems, there is a maximum freezing temperature and re-entrant melting occurs; in pure B systems, freezing to a cluster crystal phase, defined by multiple occupancy of each lattice site, occurs at all temperatures. We examine the phase behaviour in the mixture for different potential parameters. In some cases we find that the clustering behaviour of species B can induce clustering of species A in B-rich systems. We also examine the the effect of a nearby demixing transition on the properties of the crystal phases.

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Confined colloidal crystals: from bilayers to trilayers

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By lattice sum calculations of unscreened Coulomb potentials we explore the ground state phase diagram of a confined one-component plasma with a homogeneously charged background. The plasma is confined in a hard slit of width D and the background is homogenously smeared over the same slit of width D. Analytical and numerical results are obtained for single crystalline layers, bilayers and special forms of tri- and higher order layers. Similar structures have been observed experimentally.

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Equilibrium Crystal Structures for Colloidal Suspension

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Motivated by recent experiments with PMMA particles, where colloids could be designed to interact like classical hard spheres, we use a genetic algorithm to investigate the equilibrium crystal structures at zero temperature of systems having pair interactions consisting of a hard sphere interaction and various repulsive potential tails outside the core. To do so we developed a parametrisation of all crystal lattices where the hard core condition is already included to sample only configurations with non–overlapping cores using the genetic algorithm, which was necessary for good convergence. This parametrisation is presented along with results for the square shoulder potential. Despite being a rather simple example potential, it already shows a large variety of structures from clusters, lines, and lamellae to closely packed structures along the appropriate pressure range. Also the optimum structure at very high pressures, which has to be closest packed at the hard cores, exhibits a non–trivial dependency on the shoulder range, yielding structures beyond fcc and hcp.

Colloid-polymer mixtures in the presence of quenched disorder: a theoretical and computer simulation study

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We use theory and computer simulation to study the structure and phase behavior of colloid-polymer mixtures in the presence of quenched disorder. The Asakura-Oosawa model (AO) [J. Chem. Phys. **22**, 1255 (1954)] is used to describe the colloid-colloid, colloid-polymer, and polymer-polymer pair interactions. We then investigate the behavior of this model in the presence of frozen-in (quenched) obstacles. The obstacles will be placed according to two different scenarios, both of which are experimentally feasible. In the first scenario, polymers are distributed at positions drawn from an ideal gas configuration. In the second scenario, colloidal particles are distributed at positions drawn from an equilibrium hard-sphere configuration. We investigate how the unmixing transition of the AO model is affected by the type of quenched disorder. The theoretical formalism is based on the replica method of Given and Stell [Physica A **209**, 495 (1994)]. Our foremost aim is to test the accuracy of three common closures to the replica Ornstein-Zernike equations, namely, the hypernetted chain, the Percus-Yevick, and the Martinov-Sarkisov equations. The accuracy is determined by comparing to grand canonical Monte Carlo simulations. We find that, for quenched polymer disorder, all three closures perform remarkably well. However, when quenched colloid disorder is considered, i.e. the second mentioned scenario, the predictions of all three closures worsen dramatically.

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First tests on a morphological theorem for the solvation energy of non trivially shaped objects

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The solvation energy of a large solute (e.g. a colloid in a solution) depends in general in a complex way on the shape of the molecule. A morphological theorem states [1], that if some physical restrictions are imposed on the container or the solute, the grand potential depends on only four quantities, namely the volume, the surface area, the integrated mean curvature and the Euler characteristic of the container or the solute. Dumbbell shaped objects (i.e. fused spheres) are the first non trivial objects for studying the validity of the theorem. The techniques we use in our approach combine integral equation methods with density functional theory and allow us to calculate the solvation energy of large molecules. This appears to be relevant for applications of this morphological theorem to the configuration dependent solvation energy of macromolecules [2].

[1] P.-M. König, R. Roth, and K. R. Mecke, Phys. Rev. Lett. 93, 160601 (2004)
[2] R. Roth, Y. Harano, and M. Kinoshita, Phys. Rev. Lett. 97, 078101 (2006)

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Glassy Dynamics in Suspensions of Hard Ellipsoids

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We present a computer simulation study of slow dynamics in suspensions of hard ellipsoids. These systems are interesting models, in which the interplay of orientational and positional degrees of freedom can be studied. For almost spherical ellipsoids, there is a first order transition from a fluid phase to a rotator phase, i.e. a phase characterized by positional order and orientational disorder. When overcompressing the fluid phase into the rotator regime, we observe glassy dynamics both in positional and orientational degrees of freedom. This is apparent from two-step relaxation in positional and orientational correlators, and from super-Arrhenius slowing down of diffusion and relaxation. We also find that flipping modes, allowing the ellipsoids to turn upside-down, are not slowed down significantly in the studied region. We compare our results to mode-coupling theory [Letz et al., Phys. Rev. E **62**, 5173 (2000)].

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Fluctuations and pattern formation in fluids under confinement

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Competition between short-range attraction and longer-ranged repulsion in the microscopic potential is a simple mechanism leading to pattern formation in fluids even for isotropic interactions. In two-dimensional fluids, on decreasing the temperature, the particles may arrange into droplet-, stripe-, and bubble-like domains, depending on the average density. We have used numerical simulation to study the effect of confinement between two parallel walls on these microphases. For neutral walls, strong confinement changes the stripe orientation from parallel to perpendicular to the walls and, at low temperature, favors the droplet phase over the stripes. When an additional wall-particle repulsion is present, the morphology is sensitive to the details of the interactions, such as the wall-particle potential range. Studies of three-dimensional fluids by liquid-state theory show that, even when the competition between attraction and repulsion is not so strong as to suppress the bulk liquid-vapor transition, the tendency towards clustering still causes large density fluctuations in a wide region of the temperature-density plane. These affect the shape of the coexistence curve and the crossover to the critical regime as well as the long-range behavior of the correlations, which exhibit an oscillatory decay also for states close to criticality.

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Particle density dependence of electrophoretic mobilities of spherical colloids in aqueous electrolytes

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The experimental electrophoretic mobilities of colloidal charged spheres show a peculiar dependence on particle number density n in salt free and salt rich suspensions. Starting from very dilute systems, the mobility first increases, then saturates, then decreases again. Recently the high n side behaviour could be modelled by novel simulational approaches as well as by an advanced analytical theory. Both confirmed the earlier ad hoc suggestion, that at deionized conditions the particle borne counter-ions act as additional salt source. The decrease is thus understood in terms of an increased salinity. Still, the experimental observation of an increase of particle mobility with increased particle number densities at the low n side is neither backed by any standard cell model of electrophoresis with Shilov-Zharkikh boundary conditions, nor by simulation. Rather, if the experimental data are interpreted within that model an unexpected change of the zeta potential at constant added salt concentration results. Interestingly, for a Ludox suspension we observe that all experimental data collapse on a single master curve, if plotted versus the ratio C* of particle counter ions to added salt ions. We obtain a logarithmic increase of mobility for $C^* < 1$ and a plateau for $C^* > 1$. This may indicate a change of the Stern layer structure not yet included in the theoretical model.

Frederiks transition in nematic liquid crystals filled with ferroic nano-particles

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A key liquid crystalline property for electro- and magneto-optic applications is the Frederiks threshold (FT) in electric or magnetic field. The prediction in 1970 by Brochard and de Gennes [1] of the existence of magnetic colloids embedded in a liquid crystal (LC) matrix has been extremely fruitful. There has been recent experimental interest in LC-based colloidal suspensions in which the colloidal nanoparticles possess a permanent electric polarization or a permanent magnetic moment [2,3].

In recent work [4] we have examined switching properties of a ferromagnetic LC suspension in an external magnetic field in a cell with homeotropic boundary conditions. This paper considers homogeneous planar anchoring at the cell walls and ferromagnetic particle surfaces. There are three regimes, depending on the strength of the director-ferroparticle coupling. For low coupling, there is a high field inverse FT to an undistorted phase. At low non-dimensional temperatures, high magnetic fields can cause the ferromagnetic particles to segregate. Segregation-director distortion coupling can drive the inverse FT first order, causing bistability.

Here we present also further progress toward a complete theoretical model of the electric FT in a ferroelectric LC nano-suspension [5]. Using an expression for the effective dielectric tensor in ferroelectric colloids, we calculate the effect of ferroelectric impurities on the FT. We find that in some cases, even at low ferroelectric particle concentration, such doping can significantly reduce the electric FT threshold voltage.

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[3] F. Li, O. Buchnev, C.I. Cheon et al. Phys. Rev. Lett. 97, 147801 (2006).
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[5] V.Yu. Reshetnyak, S.M. Shelestiuk and T.J. Sluckin, MCLC. 454, 201 (2006).

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Dynamical density functional theory with hydrodynamic interactions and colloids in unstable traps

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A density functional theory for colloidal dynamics is presented which includes hydrodynamic interactions between the colloidal particles. The theory is applied to the dynamics of colloidal particles in an optical trap which switches periodically in time from a stable to unstable confining potential. The resulting collective breathing mode is considerably braked due to hydrodynamic interactions. The predicted dynamical density fields are in very good agreement with Brownian dynamics computer simulations.

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Lane formation in oppositely charged colloids driven by an external field

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We study a binary mixture of oppositely charged colloids which is driven by an external field by means of extensive Brownian dynamics computer simulations. The system is designed to model an experimental setup in which recently lane formation was observed. The influence of hydrodynamic interactions on lane formation is investigated using Brownian dynamics computer simulations performed on the Rotne-Prager level of the mobility tensor. Two cases are considered, namely sedimentation and electrophoresis. In the latter case the Oseen contribution to the mobility tensor is screened due to the opposite motion of counterions. The simulation results are compared to that resulting from simple Brownian dynamics where hydrodynamic interactions are neglected. For sedimentation, we find that hydrodynamic interactions strongly disfavor laning. In the steady-state of lanes, a macroscopic phase separation of lanes is observed. This is in marked contrast to the simple Brownian case where a finite size of lanes was obtained in the steady-state. For strong Coulomb interactions between the colloidal particles a lateral square lattice of oppositely driven lanes is stable similar to the simple Brownian dynamics. In an electric field, on the other hand, the behavior is found in qualitative and quantitative accordance with the case of neglected hydrodynamics.

A structural mechanism for dynamical arrest in colloidal systems

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The mechanism by which a liquid may become arrested, forming a glass or gel, is a long standing physical problem. While possible dynamic mechanisms have received considerable attention, direct experimental evidence of structural mechanisms has proved elusive. The connection between long-lived (energetically) locally favoured structures (LFS), whose geometry may prevent the system relaxing to its equilibrium state, and dynamical arrest dates back at least to F.C. Frank in the 1950s. In a similar spirit, we propose a much broader definition of LFS which we identify with a novel topological method and combine these with experiments at the single particle level on a colloidal liquid-gel transition, which we confirm with Brownian dynamics computer simulations. The population and lifetime of the LFS is a strong function of (effective) temperature in the ergodic liquid phase, rising sharply approaching dynamical arrest, and indeed the LFS form a percolating network which become the ’arms’ of the gel. Due to the LFS, the gel is unable to reach equilibrium, crystal-gas coexistence. Our results form the first direct experimental observation of a link between local structure and dynamical arrest, and open a new perspective on a wide range of metastable materials.

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Lane formation in Complex Plasmas under Microgravity Conditions

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Complex plasmas consist of charged microparticles embedded in an ordinary plasma (electrons, ions and neutral gas). Such systems can serve as suitable model systems for the description of various transport phenomena at the kinetic level (e.g., particle, momentum and energy transport in shocks, viscosity of liquid complex plasmas, heat transfer in strongly coupled (crystallized) complex plasma, diffusion in liquid, gaseous complex plasmas, etc.) In this paper we discuss experiments (PK-3 plus setup) performed aboard the ISS. Here microparticles (monodisperse melamine- formaldehyde, mass density of 1.51 g/cm^3) of different sizes were injected into a radio frequency plasma chamber, filled with Neon at a pressure of 60 Pa. The discharge was 'ignited' and driven in a parallel plate rf chamber at 13.6 MHz and a power of $\ll$ 1W. The microparticles are illuminated by a thin sheet of laser light perpendicular to the electrode system (produced by a laser diode and cylindrical optics). 15 μm and 9 μm particles form a stable complex plasma cloud with a void in the center of the chamber. When small particles of 3.4 μm are injected from the edges they penetrate through the cloud of larger particles towards the void where their trajectories stop. We observed that the small microparticles appear sometimes to simply pass through the strongly coupled complex plasma in streaming lanes without strongly affecting the structure of the penetrated cloud. Close to the void they form a drop-like cloud and move as an ensemble towards the void in the center of the chamber. We have investigated this interpenetration for different plasma parameters and are discussing the measurements and giving possible explanations for the penetration process.

P - 90

Exotic crystal superstructures of colloidal crystals in confinement

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Colloidal model systems have been used over three decades investigating the structural and dynamic properties of liquids, crystals and glasses as well as crystallization and the glass transition. Crystal superstructures have been observed in binary systems of repulsive spheres as well as oppositely charged sphere systems showing structures well known from atomic solids. We study the structural transition of colloidal crystals confined to low angle wedge geometry. Restricting the available space leads to an adaptation of the crystalline bulk structures to the symmetry of the confinement and a rich variety of structures is found as a function of colloid packing fraction and confinement dimension. In addition to the known sequence of crystalline structures, crystal superstructures with dodecagonal symmetry are observed in one component colloidal model system under confinement having no atomic counterpart.

P - 91

Magnetoactive Liquid Crystal Elastomers

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Liquid crystal elastomers (LCEs) offer an interesting spectrum of properties, including temperature induced, fully reversible shape changes connected with considerable development of pulling force, and synthetic diversity. In order to take advantage of LCEs for an extended number of viable devices, it is desirable to trigger such shape changes with electromagnetic fields rather than temperature changes. Magnetoactive LCEs are accessible by the incorporation of superparamagnetic Fe_3O_4 nanoparticles into oriented nematic side-chain LCEs and offer a contactless activation pathway to activate the nematic-to-isotrope transition by local magnetic heating in external fields due to relaxational processes. In magnetomechanical measurements at 300 kHz and 43 $kA\bullet m^{-1}$, a sample contraction of up to 30% is observed under field influence, that is fully released when the field is switched off. The load evolved reaches 60 kPa and more. The materials' ability to respond to a contactless electromagnetic stimulus with a well-defined contraction can be of use for various actuator applications.

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Ordering of colloidal particles in a 2D quasicrystalline potential

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By using Monte-Carlo simulations, we study charged-stabilized colloidal particles in a two-dimensional decagonal potential, which in experiments is realized by five interfering laser beams. We determine the phase behavior and calculate complete phase diagrams depending on the particle density and the strength of the substrate potential.

As one expects, we find a triangular to liquid phase transition for small laser intensities and a ten-fold symmetric quasicrystalline phase for high potential strengths. For intermediate intensities, however, where the colloidal ordering is influenced by both the colloidal interaction and the substrate potential, we identify a series of interesting phases: For systems with low densities, where the number of colloidal particles is less than the number of potential minima, there is a quasicrystalline phase which exhibits bond orientations in 20 different directions. When the number of colloids exceeds the occurrence of minima, we usually find a solid phase without any apparent bond-orientational order. However, for certain densities the system locks into a highly ordered phase that is close to an Archimedean tiling.

We also demonstrate how the system can be used to study the effect of phasonic distortions, fluctuations or drifts.

P - 93

The dynamics of several small rotating dumbbells in a fluid

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Dumbbells in a fluid carrying a magnetic moment may be set in rotation by an external rotating magnetic field. The hydrodynamic interaction between two or three rotating dumbbells causes a motion of the centers of mass of the dumbbells, which follow circular trajectories. The period of the circular motion of the centers of mass depends on the rotation frequency of the external magnetic flield. Transitions of three and more hydrodynamically interacting dumbbells to more complex dynamics are explored.

P - 94

Properties of colloidal suspension at the ripening process

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We report on investigations of aqueous suspensions of highly charged polystyrene spheres near the melting point. Both static light scattering and microscopy methods were employed to determine the crystal structure and the morphology. Samples were studied over extended periods of time at constant particle number densities n in the deionised state. We discuss our findings in terms of ripening in the presence or absence of uniaxial fields.

P - 95

Shear stresses of colloidal dispersions at the glass transition in equilibrium and in flow

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We consider a model dense colloidal dispersion at the glass transition, and investigate the connection between equilibrium stress fluctuations, seen in linear shear moduli, and the shear stresses under strong flow conditions far from equilibrium, viz. flow curves for finite shear rates. To this purpose thermosensitive core-shell particles consisting of a polystyrene core and a crosslinked poly(Nisopropylacrylamide)(PNIPAM) shell were synthesized. Data over an extended range in shear rates and frequencies are compared to theoretical results from integrations through transients and mode coupling approaches. The connection between non-linear rheology and glass transition is clarified. While the theoretical models semi-quantitatively fit the data taken in fluid states and the predominant elastic response of glass, a yet unaccounted dissipative mechanism is identified in glassy states.

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Vacancy Dynamics in crystals from a density functional approach

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We consider point defects in crystal in the form of mono vacancies on fcc lattice. We construct the free energy surface taking into account the presences of defects in crystals. The free energy landscape consists of a saddle which separates the two minima at corresponding to the two nearest locations of the vacancy in the crystal structure. From the free energy surface we calculate the free energy barrier height for the different densities between these two neighboring locations of the vacancy. The motion between two free energy minima represent the hopping motion of the vacancy from one lattice site to next. We have calculated the escape rate for the motion between two minima . The inverse of the escape rate is related to the Diffusion constant of point defect , and it shows activated behavior with $1/T$.

From metals to colloids: Employing the phase-field approach for ellipsoidic colloids

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The high density-phase behavior of hard ellipsoids has been studied in Monte Carlo simulations by Frenkel and Mulder in 1985. Since then, the focus of attention has been on the nematic phase and the isotropic-nematic transition. However, to our knowledge, no systematic and general understanding of the nucleation and further ordering dynamics, inclusively phase transition scenarios, is available yet. One reason is, that most simulation studies of hard ellipsoids so far, have been done based on the Monte Carlo method. This accesses time and length scales, such that the rise of individual phases, as well as their physical parameters, can be studied well. However, the successive ordering and growth dynamics, as well as the competition of different phases and related phase transitions, occurs at different time and length scales. For such approaches the phase-field approach could establish itself within the last two decades in the physical community. Lately it was shown, that this approach can also been employed to obtain the nucleation energies of homogeneous as well as heterogeneous nucleation scenarios [J. Phy. Cond. Matt. 18, 2006]. Moreover, a full dynamic coupling of a Kinetic Monte Carlo approach and a phase-field approach could be developed for epitaxial thin film growth. Thus the fundaments to apply the phase-field approach to colloids and successively couple it to obtain a multi-scale model formalism for such soft-matter systems are set. Nevertheless, available phase-field models previously obtained for metallic material systems cannot directly be applied to colloids. Rather model formulations need to be adapted switching from concentration and temperature as driving forces to a formulations based on the chemical potential as driving force. The poster elucidates the relevant steps in model derivation and depicts two different ways to employ the resulting models to gain insight in a respective colloidal model system.

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Shear induced brush deformation of soft colloids: Hybrid mesoscale simulations and Rheo-SANS experiments

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The deformation of a soft colloid by external shear fields crucially depends on its "degree of softness" and the applied Weissenberg number. ($Wi = \tau_c\dot{\gamma}$, with $\dot{\gamma}$ the applied external shear rate and τ_c the characteristic internal relaxation time of the deformable particle.)

Here we compare results obtained with multiparticle collision dynamics simulations (MPC) and Rheo-SANS experiments for dilute solutions of regular star polymers (the limiting *ultra-soft* colloid). To achieve large Weissenberg numbers we use high M_w polybutadiene (PB) star polymers dispersed in a PB oligomer matrix. We found excellent agreement between theory and experiment with respect to onset and amount of shear induced brush deformation for star polymers with varying functionality *f*.

Moreover, from MPC simulations we found that with increasing functionality star polymers exhibit a crossover in their flow properties from those of linear polymers to a novel behavior, which resembles the tank-treading motion of elastic capsules [1].

[1] M. Ripoll, R. G. Winkler, and G. Gompper, *Phys. Rev. Letters*, **96**, 188302, (2006).

P - 99

Visualization of the movement of ions in smectic films

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An experimental apparatus that comprises a freely suspended thin film of a smectic liquid crystal and an alternating electric field applied in the plane of this film allows for a direct visualization of the movement of ions in the liquid crystalline material. This is possible because a jump of the thickness of the film at the boundary of a meniscus or of a freely floating “island” is associated with a jump in the planar conductivity in the film. As a result, when ions dragged by an electrophoretic force reach the boundary their motion couples with the motion of the boundary itself and this can be visualized by optical microscopy in reflected light. Because the flow of material in thin films is subject to relatively small viscoelastic resistance we suppose that our method can be used for experimental estimation of the density of free ions in smectic liquid crystals.

P - 100

Investigation of cristallization behaviour using genetic algorithms

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When searching for new phases of star polymers and colloidal particles at zero temperature, we require an unbiased optimization algorithm heading for minima of lattice sums which would normally be difficult to predict. Several new crystal structures were found by applying genetic algorithms to attractive and repulsive potentials of star polymers and anisotropic potentials of ellipsoidal colloids. We propose methods for the enhancement of the GA’S convergence and its runtime behaviour and present algorithms to efficiently generate phase diagrams.

P - 101

Colloidal assembly on magnetically vibrated stripes.

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We investigate the collective organization of paramagnetic colloidal particles externally driven above the periodic stripes of a uniaxial ferrimagnetic garnet Film. An external Field modulation makes the stripe walls to vibrate and produces random motion of the particles. Defects in the stripe pattern break the symmetry of the potential and favor particle nucleation into large clusters above a critical density. Mismatch between particle size and pattern wavelength generates assemblies with different morphological order. By further increase the Field strength, repulsive dipolar interactions between the particles induce cluster melting. This system thus provides a novel approach to generate and externally control a variety of colloidal assemblies.

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Transport and crystallization of colloidal particles in a thin nematic cell

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In a thin planar nematic cell, the application of an AC electric field induces a macroscopic transport of micrometer-sized colloidal particles along the nematic director. We have analyzed dependence of particle velocities on the electric field amplitude and frequency and found that it decreases exponentially with increasing frequency. Using specially designed electrodes we have observed that colloidal particles could be pumped and accelerated across the field-no-field interface, and measured the structural force and the corresponding potential, which is of the order of 10000 kT for 4 μm particles. We demonstrate that spatially periodic close-packed crystalline colloidal structures can be obtained, which are thermodinamically metastable for many days after turning off the electric field and slowly decay into linear chains. Above the nematic-isotropic phase transition, such crystalline structures are non-stable and decay in few minutes.

P - 103

Rates and pathways for homogeneous nucleation under shear in a two-dimensional Ising model

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We obtain rate constants and transition paths for nucleation under shear in a two-dimensional Ising model with Metropolis Monte Carlo spin flip dynamics using forward flux sampling (FFS) simulations. We observe that the nucleation rate I shows a non-monotonic dependence on the shear rate $\dot{\gamma}$, increasing approximately linearly at low shear rates and decreasing non-linearly for high shear rates. We investigate the physical mechanisms underlying this behaviour by changing the external field strength, by randomising the shear direction and by performing a committor analysis of the transition path ensemble as a function of shear rate. We find that the enhancement of nucleation at low shear rate is due to shear-enhanced cluster coalescence, while the suppression of nucleation at high shear rates is due to shear-mediated cluster breakup. This study demonstrates the use of the recently developed forward flux sampling method for simulating rare events, including nucleation, in nonequilibrium systems and shows the highly nontrivial effect of shear on nucleation pathways in this model system.

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Goethite liquid crystalline phases in a magnetic field

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Dispersions of boardlike goethite particles form a colloidal system with interesting properties [1]. They show rich phase behaviour [2] and peculiar magnetic properties. They possess a considerable permanent magnetic moment along their long axis, presumably due to uncompensated spins within their antiferromagnetic crystal structure, combined with an induced moment with an easy axis along one of the shorter particle dimensions. Therefore, goethite particles align parallel to the magnetic field at low field strength, but they turn perpendicular to the field at high field strength.

The influence of a magnetic field on the different liquid crystalline phases has been studied by Small Angle X-ray Scattering (SAXS). A magnetic field up to 1.5 T could be applied parallel or perpendicular to the beam. Very interesting behaviour was found for the different liquid crystalline phases (isotropic, nematic, smectic A and columnar).

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[2] G. J. Vroege, D. M. E. Thies-Weesie, A. V. Petukhov, B. J. Lemaire, P. Davidson, Adv. Mater. 2006, 18, 2565.

P - 105

Two-step crystal nucleation in dilute solution

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We report Monte Carlo simulations to study the pathway of crystal nucleation from the vapor at temperatures below the triple point. Under these conditions, the Lennard-Jones system represents a simple coarse-grained model for colloids or macromolecules in dilute solution. Two distinct routes for crystal nucleation are observed: close to the triple point, surface melting can occur and a high-density liquid droplet nucleates before the crystal forms. The formation of the crystal phase involves a second nucleation step inside this droplet. At lower temperatures, we observe direct nucleation of an ordered phases. At first, small clusters with icosahedral symmetry emerge. These constitute the cores for larger twinned crystal clusters with predominantly fcc order. At intermediate temperatures, the two nucleation routes compete.

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Characterizing single colloidal particles with digital holographic microscopy

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We use in-line digital holographic[1] microscopy and Mie scattering theory to characterize and track individual colloidal particles. Each holographic snapshot provides information on the size and refractive index of hundreds of individual colloidal particles to within a few percent, while simultaneously allowing to measure the three dimensional position of the particles in the sample with nanometer accuracy, anywhere in a typical 100x100x100 μm^3 box. By studying the dynamics from multiple images we can analyze the distribution in size, refractive index, density, diffusion coefficient, sedimentation coefficient and correlations thereof.

[1] Characterizing and tracking single colloidal particles with video holographic microscopy, S.-H. Lee, Y. Roichman, G.-R. Yi, S.-H. Kim, S.-M. Yang, A. van Blaaderen, P. van Oostrum, and D. G. Grier, Optics Express 15, 18275 (2007) (www.colloid.nl)

P - 107

Colloidal crystal growth at externally imposed nucleation clusters

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We study the conditions under which and how an imposed cluster of fixed colloidal particles at prescribed positions triggers crystal nucleation from a metastable colloidal fluid. Dynamical density functional theory of freezing and Brownian dynamics simulations are applied to a two-dimensional colloidal system with dipolar interactions. The externally imposed nucleation clusters involve colloidal particles either on a rhombic lattice or along two linear arrays separated by a gap. Crystal growth occurs after the peaks of the nucleation cluster have first relaxed to a cutout of the stable bulk crystal.

P - 108

The fate of a Brownian circular swimmer

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A self-propelled Brownian colloidal rod is considered which experiences a constant force along its orientation and a constant torque. For zero temperature the resulting trajectory is a closed circle. That is why this particle is called a circle swimmer. We obtain the analytical solution for the mean position and mean-square displacement at finite temperature and discuss different regimes. We also solve the Langevin equations of motion numerically for a circle swimmer in confining channels. When placed into asymmetric channel, the Brownian swimmer can move balistically by an efficient "crawling mode" along the wall.

P - 109

Ultrasoft repulsive particles: cluster crystals in confinement

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Ultrasoft repulsive particles are known to crystallize into BCC and FCC cluster crystals [1]. Here, we study with the help of density functional theory and with simulation how a system of particles repelling each other with a simple $\exp(-r^8)$-potential (the so called GEM8-model) behaves under planar confinement. In particular, we present the phase diagram and we show how the emerging equilibrium fluid and crystal structures differ from the structures in the bulk.

[1] B. Mladek, D. Gottwald, G. Kahl, M. Neumann, and C. N. Likos, Phys. Rev. Lett. 96, 045701 (2006)

Triphasic equilibrium of charged colloidal platelets

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Charge stabilized colloidal platelets show a wide variety of liquid crystalline phases. We present a system of charge stabilized gibbsite platelets in which three phases (Isotropic, Nematic, and Columnar) coexist. The columnar phase, having the largest density, is at the bottom. The nematic phase is on top and the isotropic phase, which usually has the lowest density, is in between these two phases. Such a density inversion can take place when the platelets are highly polydisperse in size ratio (diameter/thickness). A phase diagram for this unique three phase equilibrium is proposed. During phase separation both tactoids of the nematic phase and nuclei of the columnar phase can be observed in the isotropic phase, moving in opposite directions towards their appropriate phases. The fact that the isotropic phase is in between the nematic and the columnar phase offers a unique possibility to study the formation of the columnar phase: columnar nuclei originate in the nematic phase and sediment through the isotropic phase towards the columnar phase. Results of polarization optical microscopy, transmission electron microscopy, and atomic force microscopy will be presented.

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Towards a complete band gap in the visible: epitaxial growth of binary structures

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We present easy-to-use and inexpensive techniques to make epitaxial colloidal templates, which can be used to selectively grow colloidal photonic crystals, e.g. the binary Laves structure $MgCu_2$ and the binary NaCl structure.

The $MgCu_2$ structure consists of large particles in the photonically advantageous diamond structure and small particles in the pyrochlore structure, which also recently has been identified as a good candidate for a photonic crystal with a large complete band gap in the visible [1].

The colloidal NaCl structure can also have a photonic band gap in the visible. It can be grown from a binary hard sphere dispersion. By compressing the dispersion with dielectrophoretic forces on a square hole array template, we created a thick single domain crystal.

Using templates made by time-shared optical tweezers or by lithography, and by controlling the volume fraction of the dispersion by dielectrophoresis, we can study the nucleation and growth of metastable photonic crystals from colloidal dispersions as a function of the volume fraction and the symmetry and spacing of the template.

[1] A.-P. Hynninen, J. H. J. Thijssen, E. C. M. Vermolen, M. Dijkstra, and A. van Blaaderen, Nature Materials 6, 202-205 (2007)

P - 112

Zone melting of confined driven colloidal crystals

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We report on the melt process of a colloidal charged sphere crystal confined in a long slit cell. The crystal is pushed up a stationary gradient in salt concentration by a hydrostatic pressure difference. The crystal melt interface is found beyond the freezing salt concentration, thus the crystal is overheated as long as the pushing motion is retained. The interfacial position relaxes towards the equilibrium value, once the pushing is interrupted. The experimental finding is discussed within linear screening theory and an assumed Wilson-Frenkel behaviour for reaction controlled growth.

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$[\langle x\rangle^2] \neq [\langle x\rangle]^2$

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Mixtures of colloids and polymers are interesting model systems. Even more interesting is when such a mixture is placed inside a random matrix of immobile (quenched) particles. In addition to the conventional thermal average, properties of interest now also involve an average over different disorder realizations. It then becomes possible to construct quantities like $[\langle x\rangle^2] - [\langle x\rangle]^2$, where $\langle . \rangle$ denotes the thermal average, and $[.]$ the disorder average. In the absence of quenched disorder, such a quantity would be trivially zero, but in the presence of disorder, this need not be so. In fact, on this poster, simulation evidence is provided for the existence of a divergence in one such quantity, and an important link to the random-field Ising model is uncovered.

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Beads on a Chain: Towards a New Colloidal Model System

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Using a combination of dipolar interactions induced by an external electric field and the interactions between charged particles we will show that it is possible to make linear beadsonachain starting from a dispersion of monodisperse colloidal spheres. The bonds between the spheres can be based on Van der Waals forces and/or covalent bonds. These anisotropic particles are a new colloidal model system for (bio) polymer that can be quantitatively studied in 3D real space using confocal microscopy. We will show preliminary results on how it is possible to make the beads-on-a-chain monodisperse in length and, furthermore, how it is possible to manipulate the flexibility of the chains. Moreover, the interesting phase behaviour of these systems can be used both in fundamental studies as well as to make colloidal structures that have not yet been realized.

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Elastic constants and displacement fields in crystals

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Starting with the Fourier components of the density fluctuations of a crystalline solid as broken symmetry variables the hydrodynamic equations of motion are derived. It is shown how this infinite set of equations reduce to the usual ones, if the density fluctuations are expressed in terms of a displacement field and a defect density. In the hydrodynamic limit and with the Ornstein Zernike equation of density functional theory the relation between elastic constants and the direct correlation function is shown.

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Ordered phases of block-copolymer micelles next to the solid-liquid interface

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An excellent model system for the study of crystallization in soft matter is offered by micellar solutions of tri-block copolymers, since they have well-known and rich phase diagrams. We have studied the phase behavior of the tri-block copolymer Pluronic P123 (consisting of a central part of 70 propylene oxide units terminated by two end groups of 20 ethylene oxide units) in dependence of polymer concentration and temperature.

The strong correlation of macroscopic viscosity and structural properties enables a localization of the phases using rheometry, but neutron scattering experiments are required to identify the structures involved in near-surface ordering. We performed grazing incidence small-angle neutron scattering (GISANS) measurements near the critical angle of external total reflection. To investigate the crystalline ordering in dependance on the distance to the interface the incident angle was decreased implying a high sensitivity to near-surface structures.

We observed that the chemical termination of the solid boundary influences the structure next to the interface. Furthermore an initially high structural correlation within some microns becomes markedly reduced under shear, which is in contradiction to the well-known alignment of micellar crystals under shear.

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Aggregation and hedgehog clusters of self-propelled colloidal rods in confining channels

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The non-equilibrium collective behaviour of self-propelled colloidal rods in a confining channel is studied by means of Brownian dynamics computer simulations and first-principle dynamical density functional theory. We find an aggregation of rods at the channel walls into transiently jammed clusters which exhibit a hedgehog-like structure. The microscopic theory is in qualitative agreement with the simulation data.

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The effect of solute polarizability on the hydrophobic interaction

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The interactions of macroscopic polarizable solutes in water have been studied using a computationally efficient molecular dynamic simulation methodology that we have developed. Here, the solutes are treated as generic dielectric media with a permittivity that may be systematically varied. A degree of polarization similar to the one expected in biomolecules results in dramatic changes in the hydrophobic forces between the solutes. We find that this degree of polarizability is enough to inhibit drying between hydrophobic solutes and to stabilize a reduced water density phase with a density smaller than that of bulk water. The hydrophobic forces associated with such reduced density states are still very significant with values on the order of several tens of piconewtons. Our results suggest that polarizability plays an important role in determining the hydrophobic force acting between weakly polar surfaces.

Direct observation of hydrodynamic instabilities in driven non-uniform colloidal dispersions

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The separation of bio- and macro- molecules by density gradient centrifugation is of central importance, but is limited by hydrodynamic instabilities, which lead to mixing, which suppresses and slows separation. Of fundamental interest is the connection between microscopic particle-particle and solvent-mediated interactions and the macroscopic instability. We are able to connect these two lengthscales by using tunable driven model colloidal dispersions, and have developed a means by which these instabilities may be studied systematically in real space at the single particle level. Deeper understanding of the physical mechanisms underlying mixing, and the conditions under which mixing may be suppressed, are revealed by computer simulations incorporating hydrodynamic interactions, which show quantitative agreement with experiments. We further develop a linear stability theory which captures the initial regime in which the system 'decides' whether to mix. We are thus able to make systematic predictions of conditions under which mixing occurs, with important implications for fields ranging from biology to nanotechnology.

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Computer simulations of a model colloid-polymer mixture: Equilibrium properties and critical behaviour under shear

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About 30 years ago Onuki and Kawasaki predicted theoretically that the static critical behaviour of fluids is considerably affected by external fields, e.g., shear flow. Although there is some experimental evidence that supports these predictions, a more detailed understanding can be obtained by computer simulations. Inspired by the Asakura-Oosawa (AO) model for colloid-polymer mixtures, we use WCA potentials for the colloid-colloid and colloid-polymer interactions and a very soft potential for the polymer-polymer interaction. This extension makes the model more realistic and accessible for Molecular Dynamics (MD) simulations with and without shear. Here, we introduce our model and the simulation methods, characterize its equilibrium properties and show preliminary results of the system under shear. As a first step we determine the phase diagram of the system using grandcanonical Monte Carlo (MC) simulations in conjunction with successive umbrella sampling and a cluster algorithm by Vink and Horbach, which is extended to account for continuous potentials. Structural and dynamic properties are obtained by MD simulations: The structure is characterized by the partial static structure factors from which susceptibilities and correlation lengths are extracted and compared to results of the MC simulation. With regard to dynamics, we investigate the mean square displacement and compare self- and interdiffusion constants. Finally, we show preliminary results of the susceptibilities, as obtained from MD simulations under shear.

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Transport of colloidal particles into superposition of gravity and magnetic fields

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Transport of particles in colloidal systems consisted of one type or two types of colloidal particles and accompanying phenomenons are a purpose of our investigation presented on a poster. Observing of a motion of colloidal particles, in above mentioned systems, under action of external fields we can see that its character changes in time. We can observe a transition between a state in which the particles motion is chaotic, the particles disturb each other, and a state in which the motion of them reaches some ordered, regular structures, for example lane formation phenomenon in two types colloidal system. Since these phenomenons were investigated and analysed mainly theoretically and using only computer simulations our aims is to confirm experimentally the results of these works and search some new aspects which were maybe neglected during theoretical investigation using an unsymmetrical configuration of external fields, gravity and magnetic, to drive the colloidal particles.

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