P3M algorithm for Dipolar Interactions

An extension of the P3M algorithm for dipolar interactions in three dimensional periodic boundary conditions is presented. A comparison of the computer performance
of the new algorithm with state-of-the-art dipolar-Ewald methods is done. The new algorithm
represents a substantial improvement respect current dipolar-Ewald methods. Additionally, theoretical
estimates for the root-mean square force , torque and energy errors for the real and reciprocal
space parts of the algorithm are derived. The applicability of the estimates is tested and confirmed in several numerical examples.

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Poster title: P3M algorithm for Dipolar Interactions

Charge Structure and Counterion Distribution in Hexagonal DNA Liquid Crystal

A hexagonal liquid crystal of DNA fragments (double stranded, 150 base pairs) with tetramethylammonium (TMA) counterions was investigated with small angle neutron scattering (SANS). We obtained the structure factors pertaining to the DNA and counterion density correlations with contrast matching in the water. Molecular Dynamics (MD) computer simulation of a hexagonal assembly of nine DNA molecules showed that the inter-DNA distance fluctuates with a correlation time around 2 ns and a standard deviation of 8.5 % of the interaxial spacing. The simulation also showed a distinct double layer structure, minimal effect of the fluctuations in inter-DNA distance on the radial counterion density profile, and significant penetration of the grooves by TMA. Strong counterion ordering and the absence of charge fluctuations at longer wavelengths are shown by the SANS number and charge structure factors. The DNA-counterion and counterion structure factors are interpreted with the correlation functions derived from the Poisson-Boltzmann (PB) equation and MD simulation. Best agreement is observed between the experimental structure factors and the prediction based on the PB equation. This implies that TMA is too large to penetrate the grooves to a significant extent, in contrast to what is shown by MD simulation. (by Liang Dai, Yuguang Mu,Lars NordenskiÃ¶ld,Alain Lapp,and Johan R. C. van der Maarel)

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Poster title: Charge Structure and Counterion Distribution in Hexagonal DNA Liquid Crystal

Bioceramics from Particle Stabilized Foams

Bioceramics from Particle Stabilized Foams

Franziska Krauss, Urs T. Gonzenbach, André R. Studart, Elena Tervoort, Ludwig J. Gauckler

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Aqueous foams are important in a variety of different applications ranging from food and cosmetics to oil recovery, blast mitigation, fire extinguishing and flotation processes. Well-established and emerging applications that use foams as an intermediate structure to produce macroporous materials are also widely spread in the engineering field to fabricate thermal insulating materials and low-weight structures, as well as in medicine to produce artificial implants and scaffolds for drug delivery and tissue engineering.
We present a novel and versatile method to prepare liquid ceramic foams which show unprecedented stability in the wet state. This long-term stability is achieved through the irreversible adsorption of colloidal particles at the air-water interface. The wet foam microstructure can be tailored within a wide range and high-strength porous materials can be achieved upon drying and heat treatment of the wet foams.
This method is now researched for tissue and bone scaffolds. The porous materials are aimed as porous bioceramics for cancellous bone substitution. We tailor the wet foam microstructure to meet the requirements of cell cultures such as interconnected pores with pore sizes larger than 100Âµm in order to allow the ingrowth of living tissue into the porous bone substitute.

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Poster title: Bioceramics from Particle Stabilized Foams

Synthesis of Colloidal Dumbbells

Since the work of Vinothan et al(Science 301,483,2003)there is interest in synthesizing controlled and self-assembled colloidal clusters. As well as being interesting as model systems of molecules, these clusters are also interseting for photonics because of their anisotropy. Recently in our group the synthesis of dumbbells out of colloidal silica particles was reported(Langmuir 21,11510,2005). The dumbbells are made up of 1400nm and 180nm silica particles. In my work the repreduction and development of the previous results are done and the deriving forces for the 180nm dumbbell formation is investigated.

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Poster title: Synthesis of Colloidal Dumbbells

Laning in colloidal systems of oppositely charged partilces

A recently experimentally realized set-up of oppositely charged colloidal particles is investigated with Brownian dynamic simulations. Hydrodynamic interactions (HI) are accounted for by the Rotne-Prager tensor and an Ewald-like summation of the mobillity is applied to treat the longranged part of HI.

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Poster title: Laning in colloidal systems of oppositely charged partilces

Capillary flow of dense colloidal suspensions

We analyse via confocal microscopy the behaviour of dense suspensions of colloidal spheres flowing into microchannles. Many interesting features are observed concerning the density profiles along the channels, the effects of boundary conditions on the transverse velocity profiles and the time domain of the velocity signals. In particular strong velocity fluctuations are observed and related to the local shear profiles.

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Poster title: Capillary flow of dense colloidal suspensions

Effects of the depletion interactions on the properties of a hard-rod fluid

When non-interacting polymers are added to a suspension of hard spherocylinders, the depletion forces arise between the particles. First, we used Monte Carlo simulations to look closely on the effects in the bulk and compared the obtained results with the predictions of the free volune theory. Then, we analysed changes that occured when the mixtures were confined between two hard walls.

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Poster title: Effects of the depletion interactions on the properties of a hard-rod fluid

Short charged colloidal rods

Theories on charged colloidal rods have been around since Onsager published his famous article on colloidal particles in 1949. However, these have always been applicable to long charged rods. I will discuss the possibilities in describing short charged rods in a Density Functional Theory.

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Poster title: Short charged colloidal rods

Mode selection and stretching of capillary waves by shear flow

We discuss the flattening influence of shear flow on capillary waves in a phase separated colloid-polymer system. The roughness of the colloidal gas-liquid interface in equilibrium is analytically determined from a free energy, assuming a sharp density crossover. The resulting wavevectors k that contribute to the roughness are reconsidered in the case of shear flow on the basis of the decay time of the wave, determined by the linearised Navier-Stokes equation. Waves that are slow compared to the shear rate in the same direction, are excluded from the interfacial region, resulting in a lowering of the surface roughness. From the knowledge of the equilibrium roughness, the roughness and height-height correlation function of the interface under shear flow are predicted and compared to experimental data, showing at least qualitative agreement. Expressions for the macroscopic surface tension are used to give an estimation of the contribution of the capillary waves, as well as the lower cut-off of modes, above which the theory is assumed valid.

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Talk title: Mode selection and stretching of capillary waves by shear flow
Poster title: Mode selection and stretching of capillary waves by shear flow

Electric-field-induced association of colloidal particles

In dilute aqueous suspensions of mono-disperse, micrometer-size polystyrene spheres in high frequency AC electric fields, the spheres form pearl chains oriented along the field. Using digital video microscopy, we investigate the kinetics of chain formations and the chain length distribution. Because the binding energies within each individual chain are much stronger than the interacting energies between neighboring chains, chains of a given length can be treated as a chemically distinct species. Equilibrium predictions of chain aggregation from both simulation and theory, incorporating a screened Coulombic repulsion and field induced dipole-dipole attraction, agree well with experimental results.

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Poster title: Electric-field-induced association of colloidal particles

Space dividing networks generated by two interacting species

We present a geometrical and topological analysis of cellular 'spoke' patterns observed in high Raleigh number convective instabilities. In particular, we performed experiments of solutal convection in a colloidal suspension of 11-nm silica particles in water. We show that the emerging pattern develops through the competition between two distinct cellular systems and presents some peculiar properties that clearly distinguish it from most of the 'simple' cellular systems found in nature. We develop a geometrical model for this pattern based on the Voronoi construction that, thanks to its simplicity and generality, may have a role to play in the description of others systems, in which two species of cells generators distributed across the plane interact by avoiding individuals of the other specie.

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Poster title: Space dividing networks generated by two interacting species

SIMULATIONS ON GLASSES OF HARD SPHERE

Using MC and MD simulations, we study suspensions of monodisperse and polydisperse hard spheres on the metastable fluid branch and the transition to the stable solid branch. We calculated order parameters during the crystallization and investigated the nucleation rate at different densities. All the "glass" configurations of 2000 spheres at volume fraction below 0.62 crystallize, but the crystallization rate decreases upon increasing the volume fraction towards random close packing. Preliminary comparisons with confocal microscope experiments on
PMMA colloids match very nicely.

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Poster title: SIMULATIONS ON GLASSES OF HARD SPHERE

Structural and Elastic Properties of a 2D Colloidal Binary Mixture of Magnetic Dipols

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. At high magnetic fields the system is dynamically arrested but still amorphous and 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. This is shown in a comparison of experiment, computer simulation and theory. Elastic constants of the amorphous structure are determined by measuring strain fluctuations obtained from random displacements of the particles from their mean reference positions.

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Poster title: Structural and Elastic Properties of a 2D Colloidal Binary Mixture of Magnetic Dipols

Two-dimensional colloidal crystalline structures in nematic liquid crystal

Colloidal particles confined to a few micrometer thick layer of a nematic liquid crystal form two-dimensional structures that are bound by topological defects. Two basic crystalline structures were observed, depending on the ordering of liquid crystal around the colloid. Colloids inducing quadrupolar order crystallize into weakly bound ordered chains, where the particle interaction is mediated by sharing of localized topological defects. Colloids inducing dipolar order are strongly bound into antiferroelectric-like two-dimensional crystallites of dipolar colloidal chains. The binding energies for growth procedure of crystalline structures are presented and the way of colloidal assembly is described.

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Poster title: Two-dimensional colloidal crystalline structures in nematic liquid crystal

Reversible Dialysis in a Microfluidic Formulator

In order to facilitate the screening of conditions for protein crystallization, we have been using the Microfluidic Formulator chip (Stephen Quake, PNAS Vol. 101, 40). This PDMS device allows us to mix up to 40 different reagents and protein solutions. We use this combinatorial approach along with a ``drop-on-demand'' method whereby we employ on-chip positive displacement pumps to form aqueous droplets containing protein and separate them by plugs of oil. Subsequently, the aqueous drops containing protein are guided by surface tension forces into storage chambers. To control the chemical potential of these sub-nanoliter protein samples, we fabricate reservoirs underneath the storage compartments. A thin PDMS membrane that is permeable to water, but not to protein or salt, separates the reservoirs from the storage chambers. Water can permeate into or out of the stored samples until the chemical potentials of the reservoir and the protein solution are equal leading to protein rystallization in some chambers.

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Poster title: Reversible Dialysis in a Microfluidic Formulator

Depletion-induced percolation of sticky rods

The percolation behavior of rod-like particles immersed in polymer matrices is important to achieve low-cost, conductive composites with as low as possible wt% of rods. One route to achieve this is to lower the so-called percolation threshold of the rods. There are indications that attractive interactions between rods induced, e.g., by the presence of other types of colloidal particles, can do this. Our aim is to study the connectedness percolation of sticky rods in an isotropic dispersion. One way to investigate continuum percolation is based on the connectedness analogue of the well-known Ornstein-Zernike (OZ) equation that describes the clustering behavior. An OZ relation is established between the pair-connectedness function and the direct correlation function. By the way of closure we invoke the second virial approximation. We consider a mixture of hard rods and hard spherical nanocolloids, and model the influence of the latter by an attractive depletion potential. From the analysis of the obtained expression for the mean cluster size it follows that within the effective one-component approach considered here the rods will percolate only if there is attraction between them. The attraction should be strong enough in order to create a percolating cluster of the particles. In conclusion we have considered the percolation of hard rods in the presence of spherical nanocolloids within an effective one-component approach, and confirm the attractive depletion interaction indeed lowers the percolation threshold. In future work we intend to invoke a two-component description that more accurately describes correlations in the fluid.

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Talk title: Rotational Brownian motion and light scattering by anisotropic ellipsoidal particles in a uniform dc external electric field
Poster title: Depletion-induced percolation of sticky rods

A binary Yukawa mixture under shear: A computer simulation study

Extensive Non-Equilibrium Molecular Dynamics (NEMD) simulations are performed to investigate a binary mixture of like-charged colloids under shear. The interactions between the colloidal particles are modelled by an effective screened Coulomb (or Yukawa) potential, without considering explicitly any solvent degrees of freedom. The system is coupled to a DPD thermostat while determining dynamic properties in equilibrium. The DPD thermostat is also used for the NEMD runs where the system is sheared by means of Lees-Edwards boundary conditions. We study both steady-state dynamic properties at different constant shear rates and the relaxation towards a new steady-state when the shear rate is suddenly changed. The central quantity of our analysis is the incoherent intermediate scattering function. But also structural changes are displayed by computing the static structure factors parallel and perpendicular to the direction of shear.

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Poster title: A binary Yukawa mixture under shear: A computer simulation study

Crystallisation in a 2D colloidal model system

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 positions and sizes of several thousand particles, which allows to make both statistical and local observations on all relevant length- and timescales.
The local bond-orientational order parameter makes it possible to distinguish particles in the crystal form from those in the fluid so that we can identify crystalline regions. By tracking their evolution we can observe the nucleation of colloidal crystals and grain growth in case of a temperature quench below the melting temperature. Furthermore, the behavior of defects (dislocations and disclinations), grain boundaries, and the crystal grains themselves are studied during the ripening phase.

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Poster title: Crystallisation in a 2D colloidal model system

Ultrafine Particles: a numerical model and their behavior in the absence and presence of external fields

Length scales of particles and their surrounding medium strongly
determines the nature of their interactions with one another and their responses to external fields. We are interested in systems of ultrafine particles (0.1 - 1.0 micron) such as solid aerosols, or fine powders, which are found in nature and industry. In nature, these systems are generated by volcanoes, dust storms or forest fires. In industry, they are found in pharmaceutical, cosmetic and food applications, apart from being generated by burning of fossil fuel in internal combustion engines. We present a numerical model for these systems using the Derjaguin-Muller-Toporov (DMT) theory which considers both the van der Waals attraction between the particles and their contact mechanical interactions. We study the agglomeration dynamics of these systems in the absence and presence of gravity by controlling the surface properties of the particles. Finally, we explore the response of these systems to external fields by studying the evolution of the internal microstructure under contant load and shear strain. These inquiries can be used to determine bulk material parameters such as the shear modulus and the flowability.

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Poster title: Ultrafine Particles: a numerical model and their behavior in the
absence and presence of external fields

The nonequilibrium van der Waals square gradient model for multi-component systems

K. Glavatskiy, D. Bedeaux, E. Johannessen.

The van der Waals square gradient model has been used to describe the equilibrium liquid-vapor interface. Introducing a term proportional to the square gradient of the density in the free energy density makes it possible to describe the behavior in the interfacial region at equilibrium. These systems are also observed under nonequilibrium conditions. It is therefore important to extend the equilibrium van der Waals model to the nonequilibrium case. This has been done for one-component systems. The present work extends this to multi-component systems.

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Poster title: The nonequilibrium van der Waals square gradient model for multi-component systems

Monte-Carlo simulations of a coarse-grained model for DNA-coated colloids

Colloidal particles coated with DNA with a hybridizable end group can selectively bind to colloids coated with a complementary DNA sequence. This can lead to the formation of clusters of different size. Recent experimental data on systems with two types of colloids shows strong attraction between such coated colloids, yet the size of the clusters remains finite. By means of Monte-Carlo simulations we studied the clustering of complementary coated colloids in which the DNA chains are modeled as soft colloids. When such a DNA chain bridges two colloids, it can act as an entropic spring. As a single colloid can carry many DNA chains, the model allows for the formation of large clusters but also for the formation of multiply bounded dimers. We discuss the effect of number density of polymers on cluster size and the center to center distribution functions. The results are in a good agreement with experimental observations. The distribution function of colloids always has a peak at contact distances. We find that the growth of the clusters saturates at a finite size where the steric stabilization due to the DNA inhibits further colloid addition.

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Poster title: Monte-Carlo simulations of a coarse-grained model for DNA-coated colloids

The reversible freezing and melting of colloidal crystal

We report here the observation of the reversible fluid-solid phase transition in a dilute suspension of polystyrene in 3-methylpyridine (3MP) /H2O/D2O,as approaching the coexistence
curve of binary mixture. The control parameter is the temperature.The strength and range of the interaction between the particles are tuned by the temperature. The formation of an FCC crystalline
and glass phase depend on the quenching rate. The phase behaviors are characterized by the measurement of the structure factor S(q)
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Talk title: The reversible freezing and melting of colloidal crystal
Poster title: The reversible freezing and melting of colloidal crystal

Nucleation at a pore

My poster will show how the rate of nucleation of a new phase in a pore changes with different geometries and wetting angles between the surface and nucleating phase. Chayen and her coworkers have shown that porous media are effective at inducing the nucleation of protein crystals. I show an example of how the combined rate of nucleation in and out of the pore can be optimised, and also that this rate has a maximum when the pore width is comparable to the radius of the critical nucleus. This study is performed via Ising model simulations utilizing the recently developed technique of Allen et al (1).

(1) R.J. Allen, D. Frenkel and P. R. ten Wolde
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Poster title: Nucleation at a pore

PHASE BEHAVIOUR AND PROPERTIES OF A BINARY CHARGED SPHERE SYSTEM

PHASE BEHAVIOUR AND PROPERTIES OF A BINARY CHARGED SPHERE SYSTEM
Colloidal suspensions of charged spheres play an important role as model systems for solid state physics and statistical mechanics. Their screened Coulomb interactions are conveniently varied via particle concentration and concentration of added electrolyte.
We focus on colloidal suspensions of charged spherical polymer latex in aqueous dispersion under deionized conditions. Their fluid-crystal phase transition lines including the coexistence regions can be determined by means of optical experiments. We investigate single component systems and their binary mixtures. The particles differ in size (and charge) and the phase behaviour depends on composition and total particle concentration. We find interesting deviations from the behaviour observed in random composition body centred cubic crystals. We interpret our findings in terms of an onset of compositional ordering.

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Poster title: PHASE BEHAVIOUR AND PROPERTIES OF A BINARY CHARGED SPHERE SYSTEM

Stacking disorder in hard sphere crystals

Same as presentation, only in case of rejected talk

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Talk title: Stacking disorder in hard sphere crystals
Poster title: Stacking disorder in hard sphere crystals

Widely tunable anisotropic diffusion of light in colloidal suspensions of birefringent particles

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Poster title: Widely tunable anisotropic diffusion of light in colloidal suspensions of birefringent particles

Measurement of interparticle potential in liquid crystal using magneto-optical tweezers

We used magneto-optic tweezers for measurements of liquid crystal mediated forces between microscopic beads in thin nematic samples. The main advantage of this method over optical tweezers is the low intensity of the external field used in the experiment. The magnetic field (below 10 mT) is too low to reorient the director, whereas the electric field of the trapping laser beam alters the nematic director configuration around a trapped bead [1]. We measured the force-separation dependence of the repulsive force as well as the velocity with which the particles are pushed apart by the liquid crystal [2]. The ratio yields the effective drag coefficient, which we find independent of bead separation for separations as small as 1.1-times the bead diameter.

[1] I. Musevic, M. Skarabot, D. Babic, N. Osterman, I. Poberaj, V. Nazarenko, A. Nych, Phys. Rev. Lett., 93, 187801 (2004).

[2] J. Kotar, M. Vilfan, N. Osterman, D. Babic, M. Copic, I. Poberaj, Phys. Rev. Lett., 96, 207801 (2006)

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Poster title: Measurement of interparticle potential in liquid crystal using magneto-optical tweezers

to be determined - 'Glass transitions in clay suspensions'

CargesePoster-055.data

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Poster title: to be determined - 'Glass transitions in clay suspensions'

Micro- and nano- colloids in a capillary filled with a nematic liquid crystal

Experimental and theoretical study on the ordering of micron and nano-sized colloids in a supramicrometer capillary filled with a nematic liquid crystal will be presented. With larger micron-sized colloids formation of chains is observed, which surprisingly branch in the direction perpendicular to the capillary axis. Behavior of smaller nano-sized colloids however proves to be different, since colloids either buckle together into larger Â»dropletsÂ« or form chains with various conformations.

CargesePoster-056.data

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Talk title: Micro- and nano- colloids in a capillary filled with a nematic liquid crystal
Poster title: Micro- and nano- colloids in a capillary filled with a nematic liquid crystal

Colloids dispsersed in a complex medium

The aim of my research is to study the effect of dispersed colloids on the phase diagram and phase transition kinetics of a microemulsion. Microemulsions phase separate via spinodal decomposition in a similar manner to binary fluids. The system shows a critical phase transition and has slow dynamics compared to those in binary liquid mixtures, which allowes one to study the physical processes as they happen. The dynamics are studied with optical and confocal microscopy.
In the longer term I wish to study the effect of particles on lamellar phases. Here there are lamellar phases in a solvent, and the particles can be between or in the bilayers. The addition of particles can reduce the undulation fluctuations of the bilayers or promote phase transitions. The presence of the layers can result in the particles ordering in unusual configurations.

CargesePoster-057.data

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Poster title: Colloids dispsersed in a complex medium

An exploration of applications of optical tweezers in colloid research

P.D.J. van Oostrum, A. van der Horst, A. I. Campbell, Dirk L.J. Vossen, and A. van Blaaderen

Optical tweezers are an essential tool in colloid and soft matter research because they allow exerting and measuring pN-forces in a non-invasive way, even in concentrated dispersions [1].
Tweezers can be used to create a 'line trap', creating a one-dimensional potential well for the colloids. Having two colloids on such a line and studying their positions over time is a technique to measure their pair-potential.
In addition, colloids can be trapped in 2 or 3 dimensional arrays that can act as a template to induce crystallization of other (refractive index matched) colloids. Moreover, colloids can be trapped individually to be positioned at will creating very accurate patterns. This can be done both on a glass substrate and on the edge of a crystal of colloids, with for instance different optical properties.
Analytical calculations based on a Debye-type integral representation, valid for a laser beam focused though a high numerical aperture objective as used in our setup, that yielded an explicit Mie representation of the force were performed for a wide variety of situations following a method developed in reference [2]. The outcomes of our calculations were verified by experiments. In this way the possibilities, for instance in which situations to use so-called counter propagating tweezers, were further explored and the experimental tools improved.

[1] D. L. J. Vossen, A. van der Horst, M. Dogterom, and A. van Blaaderen, Review of Scientific Instruments 75, 2960-2970 (2004)
[2] A. Mazolli, P. A. Maia Neto, and H. M. Nussensveig, Proc. R. Soc. London, Ser. A 459, 3021 (2003)

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Poster title: An exploration of applications of optical tweezers in colloid research

Slow Dynamics and Aging in Soft Colloidal Dispersions

Which is the common point between colloidal suspension, foams, emulsion and gels?
Each of this materials has a peculiar dynamics that seems vary in time and to depend strongly on mechanical history. Actually, these time-depend phenomena exhibit all the main feature of aging in glasses systems. The mechanical properties depend essentially on time elapsed after flow cessation, so-called â€˜ageâ€™ of the system. Although a lot of effort has been spent to characterize the phenomenology of aging little is know about the physical mechanism and the typical scale (nano, micro or macroscopic scale) at the origin of aging

We shall focus on concentrated dispersions of polyelectrolyte microgels that form soft glasses at high volume fraction. We studied the dynamics decay by experimental tools like the Dynamics Wave Spectroscopy, rheology or confocal microscope. We shall show how the relaxation of internal stresses and deformation locally trapped inside the materials causes aging.

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Poster title:	Slow Dynamics and Aging in Soft Colloidal Dispersions

A framework for simulations of electro-hydrodynamical problems

A framework for simulations of charged particles in solution including electrostatic as well as full hydrodynamic interactions is presented. Our approach combines different simulation methods: The hydrodynamic interactions are treated by coupling conventional molecular dynamics particles (the solute) to a Lattice Boltzmann solvent. To be able to simulate flows in channels with variable slip at the boundaries, a new boundary condition for arbitrary slip length is introduced. Electrostatic interactions can be included via the P3M method or via the Maxwell equations Molecular Dynamics algorithm. All simulation methods are implemented in the software package ESPResSo. Potential applications of the framework comprise electrophoresis and electroosmosis of charged macromolecules.

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Poster title: A framework for simulations of electro-hydrodynamical problems

Driving oppositely charged colloids with an electric field: melting and laning

Recently, we have shown that sterically stabilized PMMA-spheres suspended in an apolar organic solvent mixture can form a system of oppositely charged colloids[1]. By adding salt we can control both the particle charge and the range of the electrostatic interactions. In this way we are able to reduce the particle charges to the moderate levels needed for equilibrium phase behavior, resulting in beautiful crystals instead of aggregation. This makes it for the first time possible to grow colloidal structures resembling ionic crystals, besides entirely new structures. Here we will demonstrate the power of electric fields for manipulating these systems. A moderate field already can melt the soft crystals and it can drive the oppositely charged particles far from equilibrium in a controlled way. As a result we observe novel pattern formation, like 'laning', an out-of-equilibrium first order phase transition. Until now, this phenomenon has only been studied theoretically and in computer simulations[2], but our findings now extend the use of model colloids to this new area of strongly driven systems. With an electric field it is fairly easy to test the parameter range for which lane formation occurs and it gives the possibility to investigate time varying (oscillating) fields as well. The change in structure and dynamics can be followed quantitatively by means of confocal microscopy (in which plus and minus particles are distinguished by their different fluorescent labels) and a homemade micro-electrophoresis cell, which can be mounted on top of the microscope. We will also present preliminary investigations of the possible application of our colloidal system as electrophoretic ink or 'e-ink'.

[1] Leunissen, M.E. et al. Nature 437, 235-240 (2005)
[2] Dzubiella, J., Hoffmann, G. P. & LÃ¶wen, H. Phys. Rev. E 65, 021402 (2002)

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Poster title: Driving oppositely charged colloids with an electric field: melting and laning

CargesePoster-062.doc

The hexatic phase in a 2d colloidal system

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CargesePoster-063.doc

Sedimentation coefficient of a non-Brownian suspension

Stationary state of a non-Brownian sedimenting suspension of hard particles is studied. In particular the distribution of configurations of these particles is the main subject of interest.
A hierarchy of equations for the correlation functions, analogous to the BBGKY hierarchy known from kinetic theory, is derived and analysed for the case of a monodisperse and a polidisperse suspesnion. Next, assuming integrability of correlations, it is shown that in the low concentration limit the hierarchy can be truncated giving an equation for the two-particle correlation function. This function has been explicitly calculated, and used to compute the sedimentation coefficient. The obtained results S for a monodisperse and polidisperse (different particle radii and desities) suspensions are compared with available experimental values. Very good agreement is found.

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CargesePoster-066.doc

Nanostructured media for protein crystallisation

Piyapong Asanithi, Fiona Frehill, Alan Dalton, Joe Keddie, Naomi Chayen,Emmanuel Saridakis and Richard Sear.

One of the most important problems in the study of protein solutions is their crystallisation. Protein crystals are needed for protein structure determination via X-ray crystallography but many proteins are hard or impossible to crystallise into the large crystals needed. Crystallisation is a first-order phase transition and so proceeds via nucleation, an activated process, and growth. We have shown that bioglass, a porous medium with nanoscale pores, induces the crystallisation of a number of different proteins (Chayen, Saridakis and Sear, PNAS 2006). The poster will present these results and newer results for novel porous media engineered to induce nucleation, as well as results we have obtained that shed light in why porous media induce crystallisation. See also the poster of Amanda Page.

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Poster title: Nanostructured media for protein crystallisation

CargesePoster-067.doc

Colloidal Crystals in 2D: elasticity, structures and phase transitions

We investigate the structural and elastic properties of two dimensional colloidal systems via Monte-Carlo Computer Simulations. The colloidal systems of interest were modelled by hard disks. Simulations in the NPT- and NVT-Ensemble were carried out in order to analyse lattice formation in binary mixtures.
We also examined the influence of quenched point-like impurities on the elastic properties of a mono disperse hard disk system [1][2]. The elastic properties of these systems were calculated using a fluctuation method by S.Sengupta et.al [3].
Another point of interest is the influence of external laser fields on colloidal crystals. A binary 50% mixture with a diameter ratio of d_B/d_A=0.414 under the influence of a commensurable, spatially periodic, external laser field was analysed in this context. Simulations show that the system undergoes a laser induced phase transition, namely laser induced freezing into a S_1(AB) lattice.

[1] K.Franzrahe et. al., Comp. Phys. Commun. 169,pp 197-202 (2005);

[2] P.Nielaba, K.Binder, C.Chaudhuri, K.Franzrahe, P.Henseler, M.Lohrer, A.Ricci, S.Sengupta, W.Strepp, J. Phys.: Condens. Matter 16, S4115-S4136 (2004);

[3] S.Sengupta, P.Nielaba, M.Rao and K.Binder,Phys. Rev. E 61, pp. 1072 (2000)

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Poster title: Colloidal Crystals in 2D: elasticity, structures and phase transitions

CargesePoster-070.doc

Non Equilibrium Crystalline and Amorphous states of a Driven Solid.

We show that a collection of particles in two dimensions, interacting by an inter-atomic potential consisting of two and three body terms which supports both triangular and square crystalline states, undergoes a series of transitions when driven over a quenched random external potential [1]. Starting from a pinned square lattice, an increase of the driving force, de-pins the solid at the same time melting it. At higher values of the force, the melt crystallizes into a triangular solid, which undergoes a kinetic structural transition back to the square lattice at yet higher values of the force. We obtain the full dynamical phase diagram of the system for a range of values of the force and the strength of the three body interactions. During the structural transitions we monitor sharp changes in several quantities like transverse velocity and distribution functions for various structural and kinetic parameters. We propose to understand this phase transition in terms of a "shaking temperature" [3].

[1] A. Sengupta,S. Sengupta,G. I. Menon, Europhys. Lett. 70 (5), pp. 635-641 (2005).

[3] A.E.Koshelev,V.M.Vinokur, Phys.Rev. Lett. 73, 3580 (1994).

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CargesePoster-071.doc

Simulations on sedimentation of hard spheres

We performed simulations on hard spheres in gravity. We focused on the crystallization of the first few layers. Both the gravity and the density dependence of this phase transition were determined. The results were compared to experiments. We also calculated the lattice constant of the crystalline layers and compared it to the bulk lattice constant.

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Poster title: Simulations on sedimentation of hard spheres

CargesePoster-073.doc

Properties of trapped colloidal solids

We investigate properties of colloidal solids trapped by confining potentials. We consider several types of confinement, eg. hard and soft walls as well as laser traps in two and three dimensions which allow exchange of particles across the traps. We report unusual mechanical behaviour, and novel surface fluctuations in these confined systems. Some of these results have been already published (D. Chaudhuri and S. Sengupta, Phys. Rev. Lett. 93, 115702 (2004); A. Chaudhuri, S. Sengupta and Madan Rao, Phys. Rev. Lett. 95, 266103 (2005)) , while some of our results for trapped solids in three dimensions will be presented for the first time.

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Poster title: Properties of trapped colloidal solids

CargesePoster-079.doc

Bond-controlled dynamics of a binary mixture of hard-ellipsoid particles with attractive patchy interaction

We report on molecular dynamics simulations of hard-ellipsoid particles decorated on their surface by a predefined number M of identical short-ranged square-well attraction sites (sticky spots). The system is a mixture of big ellipsoids with M=2 and small ellipsoids with M=5, in the ratio of 5:2 that realizes an equal presence of sticky spots on the surface of the big and small particles. The site-site attractive interaction is active only between big-small particles, and each site is engaged at most in one bond. We study the case of irreversible (i.e., infinitely long-living) bond formation —by imposing an infinite barrier to be overcome in order to separate two bonded sites— at a constant packing fraction Phi=0.3 and constant temperature T=1.0. As an increasing number of bonds is formed, it is possible to observe disordered arrested states of matter in which particles are partially interconnected in a persistent network. We present results for the bond-controlled evolution of relevant static and dynamic quantities, and discuss them in connection to patchy colloids with reversible bonding, in which a decrease of T or increase of Phi is required for the establishment of a spanning network of long-living bonds between the particles. In particular, we discuss the existence of distinct arrested states of gel and glass type. The present model can be at the same time considered as a simple model for the new generation of patchy colloids or for network-forming materials obtained by polymerization.

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Poster title: Bond-controlled dynamics of a binary mixture of hard-ellipsoid particles with attractive patchy interaction

CargesePoster-080.doc

Simultaneous measurement of velocity profiles and rheology in hard-sphere glasses.

We have developed a so called 'confocal rheoscope', a combination of a cone-plate rheometer with an ultra-fast confocal microscope which images the 3D microstructure during flow through the rheometer plate. Using this instrument, we have measured velocity profiles of colloidal hard sphere glasses (index matched with fluorescent tracers) and simultaneously determined their rheological response during various rheological test. Depending on the colloid volume fraction, shear rate and coating of the cone-plate, we find different velocity profiles, ranging from linear profiles with wall slip and shear-rate dependent slip length to nonlinear, nearly exponential profiles with coexisting sheared and un-sheared regions. We discuss the relation between these results and the measured flow curves along with implications for existing data on hard-sphere rheology.

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