CPP 38: Poster: Colloids and Complex Liquids

Time: Wednesday 17:00–19:00 Location: P2

CPP 38.1 Wed 17:00 P2

Hydration and Protein Interactions in Concentrated Electrolyte Solutions Studied by SANS — •Fajun Zhang[1], Maximilian W. A. Skoda[2], Robert M. J. Jacobs[3], Philip Callow[4], Henrich Frielinghaus[5], Vitaliy Pipich[5], Sylvain Prevost[6], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]ISIS, Rutherford Appleton Laboratory, UK — [3]CRL, University of Oxford, UK — [4]Institut Laue Langevin, Grenoble, France — [5]Jülich Centre for Neutron Science at FRM II, Garching, Germany — [6]Helmholtz Center Berlin, Germany

Proteins are commonly found in relatively concentrated salt solutions during protein crystallization and purification. The exact interplay of the hydration shell, the salt ions, and protein-protein interactions under these conditions are far from understood on a fundamental level, despite the obvious practical relevance. We have studied a model globular protein (bovine serum albumin, BSA) in concentrated salt solutions by SANS. By comparing with previous studies using SAXS [1], a hydration level of 0.37 g/g protein is determined. The forward intensity determined from Guinier analysis is used to determine the second virial coefficient, A_2, which describes the overall protein interactions in solution. It is found that A_2 follows the reverse order of the Hofmeister series. These effects are further discussed by comparing the contribution from the excluded volume. SANS data are further analyzed on the full q-range using liquid theoretical approaches, which is consistent with A_2 and the experimental structure factor. [1] F. Zhang, et al., J. Phys. Chem. B 2007, 111, 251.

CPP 38.2 Wed 17:00 P2

Static and Dynamic Crowding Effects from Charge- to Sterically Stabilized Protein Solutions — •Fabio Zanini[1,3], Marco Heinen[2], Felix Roosen-Runge[1], Fajun Zhang[1], Marcus Hennig[1,3], Tilo Seydel[3], Gerhard Nägele[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, Jülich, Germany — [3]Institut Laue Langevin, Grenoble, France

We have investigated static and dynamic properties of aqueous solutions of bovine serum albumin (BSA) in an integrated conceptual framework, combining static and dynamic light scattering (SLS/DLS) and small-angle X-ray scattering (SAXS) with colloid theory. We focus on solutions with sodium and calcium chloride, which are physiologically relevant and well-suited for effective modelling. Using a new theoretical approach, we are able to reproduce the measured collective diffusion constant and structure factor, up to volume fractions of 5-10% [1]. By tuning the ionic strength, we quantify the effect of macromolecular crowding along the crossover from charge- to sterically stabilized protein solutions. Moreover, we test the validity of various generalized Stokes-Einstein equations (GSE), which connect osmotic compressibility, diffusion constant, and viscosity of complex liquids. We find that, despite their appealing simplicity, the GSE schemes fail to capture the essential richness of macromolecular collective diffusion. [1] M. Heinen *et al.*, J. Appl. Cryst., 2010, 43, 970-980.

CPP 38.3 Wed 17:00 P2

Pressure Dependence of the Interaction Potential of Protein Solutions — •Martin Schroer[1], Jonas Markgraf[2], Florian Wieland[1], Christoph Sahle[1], Johannes Möller[1], Michael Paulus[1], Metin Tolan[1], and Roland Winter[2] — [1]Fakultät Physik / DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund (Germany) — [2]Fakultät Chemie, Physikalische Chemie I, TU Dortmund, Otto-Hahn Str. 6, 44227 Dortmund (Germany)

Pressure, one of the fundamental thermodynamic variables, allows to change in a controlled and reversible way the intermolecular interactions of proteins in solution without the major perturbations produced by changes in temperature or chemical composition. Moreover, hydrostatic pressures are also relevant for understanding life under extreme conditions, as for instance in exobiological or deep sea environments (where organisms have to cope with pressures up to ~1 kbar). Hence, studying protein-protein interaction as a function of pressure will give a deeper insight into the high stability of dense protein solutions (as they occur intracellularly) in biosystems living under hydrostatic pressure conditions. We present recent results of the influence of pressure on the structure and protein-protein interaction potential of dense protein solutions studied using small angle X-ray scattering (SAXS).

CPP 38.4 Wed 17:00 P2

Small Angle Scattering of Triglyceride Nanosuspensions — •Martin Schmiele[1] and Tobias Unruh[2] — [1]Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM-II), Lichtenbergstr. 1, D-85747 Garching — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Kristallographie und Strukturphysik, Staudtstraße 3, D-91058 Erlangen

Colloidal suspensions of triglyceride nanocrystals are considered as potential drug delivery carriers in modern pharmaceutical technology. The main focus of our group lies on tripalmitin nanocrystals stabilized with phospholipids in an aqueous dispersion medium. While the mesoscopic structure of such dispersions is well studied [1] the structure of the stabilizer layer in the interface between the particles and the dispersion medium is not. It will be demonstrated that it is possible to gain detailed information about the structure of the stabilizer layer by simultaneous analysis of SAXS and SANS data. For this purpose the X-ray powder pattern simulation analysis [2] was extended to be used for neutron data as well. In the talk the simulation method will be introduced and a comparison of recent experimental and simulation results will be presented. [1] T. Unruh, H. Bunjes, K. Westesen, M.H.J. Koch. Colloid Polym. Sci. 279, 398 (2001) [2] T. Unruh. J. Appl. Cryst. 40, 1008 (2007)

CPP 38.5 Wed 17:00 P2

Experimental Observation of Colloidal Micelles — •Daniela Kraft[1], Ran Ni[2], Michiel Hermes[2], Kisun Yoon[3], David Weitz[3], Alfons van Blaaderen[2], Marjolein Dijkstra[2], and Willem Kegel[1] — [1]Van't Hoff Laboratory for Physical and Colloid Chemistry, Debye Institute for NanoMaterials Science, Utrecht University, The Netherlands — [2]Soft Condensed Matter Group, Debye Institute for NanoMaterials Science, Utrecht University, The Netherlands — [3]Experimental Soft Condensed Matter Group, SEAS, Harvard University, USA

Colloidal particles have often been used as analogues of atoms for studying for example crystallization and are widely anticipated as ideal candidates in bottom-up assemblies with rationally designed properties. So far, super-structures such as crystals were determined mainly by the particle shape due to centrosymmetric interactions. Site-specific interactions, so called patchy interactions, between colloids may open up new and exciting assembly possibilities.

Here, we present an experimental realization of such site-specific patchy attractions between complex colloids through depletion interactions, and apply the technique to the most simple case of colloids with one patch. Such colloids with one attractive patch form clusters that resemble surfactant micelles. We discuss the similarities between the observed colloidal clusters and surfactant micelles and compare the results to computer simulations. A theoretical micelle model is used to quantify the results.

CPP 38.6 Wed 17:00 P2

Forces of Interaction within Single Pairs of Polymer-grafted Colloids as Measured by Optical Tweezers — •Mahdy M. Elmahdy[1,3], Alla Synytska[2], Christof Gutsche[1], Gustavo Dominguez-Espinosa[1], Astrid Drechsler[2], Petra Uhlmann[2], Manfred Stamm[2], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, Germany — [2]Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden, Germany — [3]Department of Physics, Mansoura University, Mansoura 35516, Egypt

Optical Tweezers are ideal tools to measure the interaction forces between polyelectrolyte-grafted colloids. Using this technique, the forces of interaction within single pairs of poly(acrylic acid) (PAA) and poly(2-vinylpyridine) (P2VP)-grafted colloids are measured as a function of concentration, valency as well as pH of the surrounding medium [1,2]. The PAA- and P2VP-grafted colloids data are quantitatively described by the Jusufi model for spherical polyelectrolyte brushes. The transition from an osmotic to the salted brush regime is observed in both polyelectrolytes. In the salted brush regime, power law dependence with an exponent of 0.3 is found, in good agreement with scaling laws. For the PAA-grafted colloids, the brush height increases with increasing pH while the P2VP-grafted colloids show a transformation in the conformation of the brushes.

References [1] Elmahdy et al., Macromolecules 2009, 42, 9096. [2] Dominguez et al., Polymer 2008, 49, 4802.

CPP 38.7 Wed 17:00 P2

Confocal Microscopy of Colloidal Aggregates under Shearing — •Jennifer Wenzl, Miao Wang, Marcel Roth, and Günter K. Auernhammer — Max-Plack Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz

Colloidal dispersions show a rich variety of phenomena and can therefore also act as model systems for granular matter. To infer the macroscopic behavior of granular material from interactions between single particles, detailed informations about the mechanical and structural properties are necessary. This is realized in particular with a large translational shear between parallel plates with simultaneous observation by a confocal microscope. Therewith we obtain three dimensional coordinates and trajectories of every particle in the imaged volume with high resolution. The shearing is done via a piezo-controlled cell, which enables the positioning of the shear plates with nanometer accuracy. The sample thickness is variable up to 160 μm on a micrometer scale and can be verified by confocal images. As a model system we use fluorescent core-shell silica particles in cis-decaline, as they show a weak aggregation. In this presentation we address the following questions. How do particles or aggregates deform under shear or compression? Do particles slide past each other or do they roll off under external shearing forces? How are forces transmitted in colloidal films?

CPP 38.8 Wed 17:00 P2

Micro-rheology on colloids using Optical Tweezers — •Christof Gutsche, Tim Stangner, Mahdy M. Elmahdy, Olaf Ueberschär, Carolin Wagner, and Friedrich Kremer — Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, Germany

Optical tweezers are experimental tools with extraordinary resolution in positioning (+/- 2 nm) a micron-sized colloid and in the measurement of forces (approx. 50 fN) acting on it - without any mechanical contact. This enables one to carry out a multifold of novel experiments. In the following forces within single pairs of colloids in media of varying concentration and valency of the surrounding ionic solution will be presented.

CPP 38.9 Wed 17:00 P2

Interactions between polymers and curved surfactant layers — •Andreas Weber, Shun Yu, Tinka Spehr, and Bernd Stühn — Institut für Festkörperphysik, TU Darmstadt

We study the interaction between polymers and curved surfactant layers in microemulsions in the droplet phase, where surfactant stabilized droplets of water are dispersed in a matrix of oil. To study the difference between ionic and non-ionic surfactants we use either an ionic surfactant (AOT) or a non-ionic surfactant (C12E5, Brij®30). First, we examine the phase diagram of water-in-oil droplets without polymer. This is done by small angle X-ray scattering (SAXS) and light transmission experiments, where the turbidity point and thus the stability of the microemulsion is measured as a function of temperature. Then, to investigate the interaction between polymer and the curved surfactant layer, we add the hydrophilic polymer Polyethylene glycol (PEG). The location of the PEG inside the droplet is predicted to depend on the nature of the surfactant: While the PEG is expected to adsorb to the layer of the ionic surfactant AOT, in non-ionic microemulsions the PEG is supposed to be located in the water core away from the surfactant layer. SAXS is used to investigate the structure of the polymer loaded micelles and possible deformations of the droplets, dynamic light scattering and dielectric spectroscopy provide information concerning the dynamics of the droplets and the surfactant interface.

CPP 38.10 Wed 17:00 P2

Efficiency boosting in application: The influence of Poloxamers on skin friendly microemulsions for decontamination — •Sebastian Höhn[1], Ralph Neubauer[1], Christoph Schulreich[1], and Thomas Hellweg[2] — [1]Physikalische Cemie 1, Universität Bayreuth, Deutschland — [2]Physikalisch und Biophysikalische Chemie (PC III), Universität Bielefeld, Deutschland

Bicontinuous microemulsions based on sugar surfactants are the promising media for decontamination. Various toxic chemicals and most chemical warfare agents are hydrophobic while most degradation agents are hydrophilic. Microemulsions offer an oil and a water phase, separated by a huge internal interface which allows interaction of the enzymes with the warefare agents. One limiting factor for applications is the high demand of surfactant to form stable microemulsions. By adding small amounts of amphiphilic diblock copolymers the surfactant efficiency is dramatically enhanced (efficiency boosting effect). In this contribution the influence of different commercially available triblock copolymers (Poloxamers) on two systems is shown. Due to the fact, that the added block copolymers are part of the amphiphilic interface, where the decontamination takes place the influence of different polymers on the interfacial film is of high interest. Therefore, we investigate the model system based on n-decyl-β-D-maltoside ($C_{10}G_2$) and cyclohexane by SAXS and SANS. In order to compare this model system with a technical system we changed to Simulsol SL55 ($C_{10-12}G_{1.3}$, Seppic). Upon addition of small amounts of poloxamer an increase of the surfactant efficiency is observed.

CPP 38.11 Wed 17:00 P2

Water in Reverse Micelles Studied by Neutron Scattering — •Tinka Spehr[1], Bernhard Frick[2], Isabelle Grillo[2], and Bernd Stühn[1] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut Laue-Langevin, Grenoble, France

We performed neutron scattering studies on water-in-oil droplet microemulsions based on the anionic surfactant AOT to investigate the effect of micelle size on the dynamics of water. First we studied the structure and the self dynamics of the droplets as a function of temperature and composition. Using small-angle neutron scattering and elastic scans on neutron backscattering (BS) we characterized the microemulsion structure and its stability. We find that the droplets are stable down to temperatures where the contained water is deeply supercooled [1],[2]. Neutron-spin-echo was then used to determine the bending elasticity of the surfactant film and the diffusion coefficient of the entire droplets in the oil matrix [2]. Finally we focussed on the water dynamics inside droplets of two different sizes, $\omega = 3$ (8) corresponding to $R = 7$ (12) Å, combining neutron time-of-flight and BS. The average mobility of the confined water is slowed down compared to bulk water. Inside bigger droplets we observed two dynamically separated water fractions - probably corresponding to bound shell water and bulk-like core water - whereas in smaller droplets all water appears to be closely bound [3]. Wide-angle X-ray scattering is used to monitor ice formation inside the droplets. [1] T. Spehr *et al.*, Phys. Rev. E **79** (2009), 031404; [2] T. Spehr *et al.*, J. Phys.: Condens. Matter **20** (2008), 104204; [3] T. Spehr, PhD Thesis, TU Darmstadt (2010)

CPP 38.12 Wed 17:00 P2

Transparent superhydrophobis surfaces made out of hybrid raspberry-like particles — •Doris Vollmer, Maria d'Acunzi, Lena Mammen, Xu Deng, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research

We report a novel method to prepare superhydrophobic films from raspberry-like particles. The term raspberry refers to the topography of the surface of the hybrid particles, which consists of a micrometer-sized polystyrene core and a rough silica shell. Multilayers of particles are formed by evaporation of the aqueous dispersant. Mechanical stability can, for example, be induced by exposure of the multilayer to a good solvent for the polymer core. Polystyrene leaks out of the core and forms bridges between the particles. The films are hydrophobized by silanization with a semifluorinate silane. Films show static contact angle for water of about 160° and roll-off angle of a few degree. Furthermore, we discuss the mechanical stability of the coatings and show how to render them transparent.

D'Acunzi, L. Mammen, M. Singh, X. Deng, M. Roth, G.K. Auernhammer, H.-J. Butt, and D. Vollmer, Faraday Discussion, 146, 35-48, 2010

CPP 38.13 Wed 17:00 P2

Hydrodynamics of colloidal suspension under external force in a narrow channel in 2D — •Fatemeh Tabatabaei — Institute for Solid State, Research Center Juelich, 52428 Juelich, Germany

Investigating biological or chemical systems which are consist of particles under different degrees of confinement has got great interest recently. In this work we study a suspensions of disc-like particles between two planar walls by means of simulation. The system under influence of sedimentation along the walls as an external force is considered. The settling speed of a colloid in respect to varying geometrical parameters are calculated. By calculation of velocity profile of the fluid particles, the effect of Hydrodynamic interaction due to solvent's flow in the laminar regime is discussed. In the next step the dependency of the sedimentation velocity on the volume fraction of colloidal particles is considered. Here a hybrid simulation scheme which couples a Molecular dynamic simulation method to a multi-particle-collision (MPC) fluid is used. This is a coarse-grained model to describe fluid dynamics.

CPP 38.14 Wed 17:00 P2

Supramolecular structure changes of tubular J-aggregates on various substrates upon drying from water — •Chien-Lie Lee, Dörthe M. Eisele, Stefan Kirstein, and Jürgen P. Rabe — Humboldt-Universität zu Berlin, Germany

Tubular J-aggregates self-assemble from amphiphilic cyanine dyes in aqueous solution. Although the main driving force for the self assembly results from the hydrophobic effect there are other contributions to the cohesion of the molecules. Therefore, it is possible to transfer these aggregates onto solid substrates where they remain intact, without substantial changes of the morphological and supramolecular structure, as long as as the samples are not completely dried [1].

Here we investigate the role of the hydrophilicity or hydrophobicity of the substrate on the drying and hence destruction of the aggregate structure. The high sensitivity of the optical spectra to changes of the molecular packing within the J-aggregates is used to probe the structure. The hydrophilicity of the substrate is controlled by coating with polyelectrolyte or polymer layers and the drying of the aggregates is recorded time dependent and under controlled humidity.

[1] D.M. Eisele, J. Knoester, S. Kirstein, J.P. Rabe and D.A. Vanden Bout, Nature Nanotech. 4 (2009) 658;

CPP 38.15 Wed 17:00 P2

Self - Assembly of Two Dimensional Ordered Arrays of Mesoscopic Particles on Solid Surfaces — •Züleyha Yenice and Regine von Klitzing — Technische Universität Berlin, Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Sekr. TC 9 Straße des 17. Juni 124 D - 10623 Berlin

Self-assembled two-dimensional (2D) colloidal crystals with submicrometer-scale periodicity are of considerable fundamental and technological importance in nanosphere lithography, optical devices, data storage and biosensors as well as model systems for 2D crystallization.

The objective of the current research is to control the distance between particles in a 2D lattice [1]. The deposition of the particles on to the wafer is accruing by spin coating technique. Here the effect of different rotational speed, type of solvent and different concentrations of the particles in the suspension were examined. For morphological observation an atomic force microscope (AFM) operating in the tapping mode was used. However, there is a lack of information about the preparation of high ordered colloidal arrays with the interparticle distance.

References [1] P. Jiang, M. J. McFarland. J. Am Chem. Soc. 2004,126, 13778-13786

CPP 38.16 Wed 17:00 P2

Bicontinuous microemulsions at solid surfaces — •Stefan Wellert[1], Ralf Stehle[2], Christoph Schulreich[3], Roland Steitz[2], and Thomas Hellweg[3] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Inst. f. Chemie TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin — [2]Helmholtz Zentrum Berlin, Hahn-Meitner Platz 1, D-14109 Berlin — [3]Universität Bielefeld, Physikalische und Biophysikalische Chemie (PC III) Universitätsstr. 25, D-33615 Bielefeld

The commercial availability of a large variety of bioinspired surfactants results in a renewed interest in microemulsions being thermodynamically stable self-assembled structures of oil, water and amphiphiles.

Solid surfaces play an essential role in many desired applications. The involved real surfaces can be of variable hydrophobicity due to external influences (e.g. weathering) leading to continuously modified physico-chemical properties of these surfaces. Especially bicontinuous microemulsions are of great interest and the physico-chemical properties of these structure in the bulk phase were studied in many surfactant systems but much less is known about the behaviour or changes of this structure in the presence of a solid surface.

Neutron reflectometry is well suited to resolve the structure of the interface between the microemulsion and the solid surface and we report on measurements on bicontinuous structures on hydrophilic and hydrophobic surfaces. Additionally, we discuss the wetting properties in terms of contact angles at different oil-water ratios at hydrophilic, -phobic and partially hydrophobic surfaces.

CPP 38.17 Wed 17:00 P2

Interactions between geometric defects in 2D colloidal systems — •David Polster, Georg Maret, and Peter Keim — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

Melting in 2D, according to the Kosterlitz-Thouless-Halperin-Nelson-Young theory, involves the formation and dissociation of topological defect pairs. Because these defects distort the hexagonal symmetric of the 2D crystal it is not possible that an isolated topological point defect is formed. Consequently, topological defects occur always as dislocation or disclination pairs.

Geometric defects on the other hand are isolated point defects which can experimentally created e.g. with an optical tweezer. While topological defects appear already near kT geometric defects need a lot more energy to create. We study the interactions of geometric defects with other defects or the surrounding undisturbed lattice in a 2D system of paramagnetic colloidal particles which are sediment to a water/air-interface. By applying a magnetic field the particles form a 2D crystal with hexagonal symmetry which can be manipulated with an optical tweezer. Thereby, we are interested as well in vacancies as in interstitials. First is created by remove a colloidal particle, second by draw a particle into the crystal.

CPP 38.18 Wed 17:00 P2

Confined Binary Colloidal Crystals in 2D: Monte Carlo Simulation of Crack Formation — •Stefan Medina Hernando, Peter Virnau, and Kurt Binder — Institut für Physik, Uni Mainz, Germany

As recent studies have shown, the confinement of a two-dimensional strip of a binary (A,B) colloidal mixture by walls in one direction may either stabilize or destabilize the crystalline structure depending on the type of wall. However, an introduction of misfit, i.e. a reduction of space between the walls, leads to the appearance of grain boundaries in both cases. These crack patterns typically have a width of several particle diameters and, depending on the extent of the misfit, are spread over the colloidal strip. Large misfits may even drive the system into a glassy state. We also present various methods to characterize order and disorder in such systems.

CPP 38.19 Wed 17:00 P2

Diffusion of amphiphiles and proteins in the bicontinuous phase of a microemulsion: A fluorescence correlation spectroscopy study — •Ralph Neubauer[1], Sebastian Höhn[1], Christoph Schulreich[1], and Thomas Hellweg[2] — [1]Physikalische Chemie I, Universität Bayreuth, Deutschland — [2]Physikalische und Biophysikalische Chemie (PC III), Universität Bielefeld, Deutschland

The bicontinuous phase in a microemulsion is often characterized by dynamic light scattering (DLS) or small angle neutron scattering (SANS). Here we analyze the diffusion of a bicontinuous phase by fluorescence correlation spectroscopy (FCS) to determine the diffusion time and coefficient of tracer particles. FCS is a powerful technique for obtaining readings and results much faster than in an DLS experiment.

In the present work fluorescein labeled amphiphilic molecules are inserted in the microemulsion. By measuring the diffusion of the amphiphiles, the "breathing movement" of the interface layer can be identified. Furthermore, the movement of fluorescent labeled proteins in the water domain is detected and the confinement effect can be identified.

Moreover we compare results from different DLS, SANS and FCS measurements for the bicontinuous phase of sugar surfactant based microemulsions. We also show conclusions for model systems and corresponding systems with technical-grade surfactants. The challenge especially for technical-grade systems is the fluorescence of impurities in the surfactants all over the visible range which cannot be extinguished.

CPP 38.20 Wed 17:00 P2

Crystallization of charged colloids in extreme confinement — •Tetyana Kromer-Vovk, Nadezhda Gribova, and Axel Arnold — ICP, Universität Stuttgart, Germany

Freezing effects in spatially confined fluids and colloidal dispersions receive strong scientific interest over the last decades. Confining surfaces can be found in many contexts like the inner walls of porous materials or in a blood cell. In 3D freezing is a first-order phase transition between liquid and solid phase, while the phase behavior in 2D systems is more complicated since no real long-range translational order exists. The theory predicts a hexatic phase with short-range translational and quasi-long orientational order between liquid and solid. Although several works reported the existence of a hexatic phase in such systems, there still remains debate on the exact nature of the transition.

In our work we present MD simulations of a system of charged colloids in confinement using the ESPResSo software package. We investigated the phase behavior of a two layers system confined between parallel neutral walls. We studied various parameters to check for the presence of a hexatic phase. We find practically no energy barrier to nucleation, clearly showing that the freezing behavior differs from the bulk nucleation scenario. However, instead of an intermediate hexatic phase we find only a region of pronounced crystal-liquid coexistence. We also investigate the influence of various fixed crystal seeds as templates for the crystal phase. The seed enhances the phase separation and through this gives the impression of nucleation around the seed.

CPP 38.21 Wed 17:00 P2

Like-charge attraction in confined colloidal systems — •Dmitriy Rozhkov[1], Sofia Kantorovich[1,2], and Marcello Sega[2] — [1]Ural State University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]Institute fuer Computerphysik, Universitaet Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Deutschland

In Ref. [1] it was shown that DNA molecules in aqueous solution stretched spontaneously along the walls of a glass nanochannel. The attraction of negatively charged spherical colloidal particles to the wedges was also observed. Both effects seem surprising as they demonstrate the attraction of likely charged objects in presence of monovalent salt. At the moment there is no definitive explanation for this effect. Here we use molecular dynamic simulations performed using ESPresSo [2] in order to elucidate the problem using a model system, composed by one colloidal particle and monovalent salt at different concentrations. The results of molecular dynamics simulations are also compared to the solution of the Poisson Boltzmann equation.

[1] M. Krishnan et al, Nano Lett., 7 (5) 1270 (2007) [2] H-J Limbach et al, Comput. Phys. Commun. 174(9) (704-727), 2006

CPP 38.22 Wed 17:00 P2

AFM study on the structuring of silica nanoparticles in confined geometries — •Yan Zeng, Sebastian Schön, and Regine von Klitzing — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Strasse des 17.Juni 124, D-10623 Berlin

Colloidal suspensions are omnipresent in daily life and have many technical applications. To understand the interactions between particles in thin films of colloidal suspensions, we perform force measurements by using Colloidal Probe Atomic Force Microscopy (CP-AFM), in which particles show oscillatory force due to the layer formations of particles under spatial confinement.

Previous works have been done in the field of the effect of particle concentration, particle size and ionic strength on the structuring of the Ludox silica nanoparticles between two rigid confining surfaces. The layer-layer distance in the confined geometry is compared with the mean particle distance from the corresponding free volume case with Small Angle X-Ray Scattering (SAXS).

To understand the effect of confining surfaces properties on the structuring of the nanoparticles in between, confining surfaces are modified thus different surface charge, surface roughness and surface elasticity are obtained. In addition, the adsorption of surfactants on the surface of nanoparticles are studied as well.

CPP 38.23 Wed 17:00 P2

Percolation transition of colloids with short-ranged attraction in a slit-pore geometry. — •Helge Neitsch and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We have performed event-driven molecular dynamic (EDMD) simulations of a system consisting of colloidal particles with ultra-short ranged attractive interactions which are confined by two smooth, parallel walls. The pair-wise interaction between the particles is modeled using a square-well potential with an attraction length of 4% of the particle diameter. In the present system we investigate structural and dynamical properties via quantities like cluster-mass distributions and mean square displacements for the bulk and the confined system using wall distances down to two particle diameters. Above the metastable liquid-liquid spinodal, which has been estimated for the bulk system and all given wall distances, a percolation transition has been found even in the case with the lowest wall distance.

CPP 38.24 Wed 17:00 P2

Exploring the deposition conditions for formation of larger colloidal arrays. — •Matthias Schwartzkopf, Mottakin M. Abul Kashem, Andrew Akbashev, Adeline Buffet, Gerd Herzog, Jessica Lucénius, Jan Perlich, Stephan V. Roth, and Rainer Gehrke — HASYLAB at DESY, Notkestr. 85, D-22603, Hamburg, Germany

Installing regular arrays on mesoscopic length scales plays an important role in nanotechnology. Different techniques of self-assembly via solvent evaporation out of dispersions have been used to obtain highly ordered colloidal structures [Roth]. We used Langmuir-Blodgett (LB) technique and spray deposition [Buffet], representing the most attractive tools for the formation of larger homogeneous colloidal arrays on any kind and shape of substrate. Due to their different deposition and boundary conditions, the assembly behaviour of polystyrene nanoparticles changes, resulting in two-dimensional layers with LB-technique and a large variety of pattern by spray deposition. We present our first results from atomic force microscopy and microbeam grazing incidence small-angle x-ray scattering (*GISAXS).

[Buffet] AEM 2010 accepted
[Roth] APL 2007

CPP 38.25 Wed 17:00 P2

Critical Casimir Forces in Colloidal Suspensions of Janus Particles — •Olga Zvyagolskaya[1] and Clemens Bechinger[1,2] — [1]Universität Stuttgart — [2]Max-Planck-Institut für Metallforschung, Stuttgart

We investigate the behavior of a two-dimensional colloidal system of Janus particles immersed in a critical binary liquid mixture of water and 2,6-lutidine. Janus particles, i.e. particles with antipodal preferential adsorption properties for the two components of the mixture were created by silica particles with a chemical anisotropy. Close to the critical point, critical Casimir forces arise between the particles whose amplitude and sign strongly depend on the temperature and the relative particle orientation. Due to the strong non-isotropic character of these forces, we observe a large variety of colloidal structures in such systems.

CPP 38.26 Wed 17:00 P2

Coupled colloidal particles out of equilibrium — •Carmen Groben[1], Valentin Blickle[1], Jakob Mehl[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — [2]Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart

During the last two decades, there has been considerable progress in the understanding of thermodynamic processes in microscopic systems, where thermal fluctuations cannot be neglected. In this novel field of microscopic thermodynamics, experiments using single colloidal particles play an essential role, since there the phase-space trajectory can be directly observed optically.

To analyse more realistic situations, we extend a well-established single particle technique to study multiparticle nonequilibrium systems. Using rotating laser tweezers, we create two independent nonequilibrium steady states (NESS). Each NESS consists of a single superparamagnetic colloidal particle circulating in a three-dimensional toroidal laser trap. When magnetizing the particles by an external magnetic field, we induce a magnetic dipole-dipole interaction and therefore the coupling between the two NESS becomes adjustable. Depending on the driving forces and the magnetic coupling, we observe large differences in the trajectories of the particles. In our analysis we focus on the effective diffusion coefficient, which exhibits a maximum as a function of the coupling strength.

CPP 38.27 Wed 17:00 P2

The isotope Soret effect in molecular liquids: a quantum effect at room temperatures — •Steffen Hartmann[1], Konstantin Morozov[2], Zina Slimane[1], and Werner Köhler[1] — [1]Physikalisches Institut, Universität Bayreuth — [2]Department of Chemical Engineering, Technion - Israel Institute of Technology, Haifa

In a multicomponent system, a temperature gradient induces a diffusive mass flow, which is counterbalanced in the stationary state by

Fickian mass diffusion. The occuring concentration gradient can be described by the Soret coefficient, which can be split into additive contributions. We have developed a theory for the so-called isotopic contribution to the Soret effect of binary liquid mixtures based on the contribution of librational and vibrational motions to the partial pressure. Contrary to its name, the isotopic contribution is not limited to purely isotopic substitution but can be dominating or even sole effect in mixtures of different but chemically similar molecules. To test the theory, we have performed experiments for the binary mixtures from the homologous series of the halobenzenes and for halobenzenes in toluene and cyclohexane, respectively.

CPP 38.28 Wed 17:00 P2

Multicomponent diffusion in microgravity environment — •Matthias Gebhardt, Andreas Königer, and Werner Köhler — Physikalisches Institut, Universität Bayreuth

In particular transport processes in true multicomponent systems (n > 2) are still not fully understood and there is a lack of experimental data for ternary and higher mixtures. In many cases the Soret cell, where a liquid sample is placed between two differentially heated copper plates, is used in experiments. The absence of convection is crucial for purely diffusive heat and mass transfer. It is known that many liquids can exhibit negative separation ratios, i.e. heavier components segregate to the hot regions. In gravity fields this has a destabilizing effect on the system and can cause convective instabilities. Microgravity experiments (TRIMIX) are planned using the SODI facility onboard the ISS, which is equipped with a two-color Mach-Zehnder interferometer. We are performing accompanying ground based measurements using a two-color optical beam deflection technique. We provide first experimental results and discuss the influence of the refractive index dispersion relations on the feasibility of the experiments.

CPP 38.29 Wed 17:00 P2

Dispersion study of Carbon Nanotubes — •Gerhard Lackner[1], Viktor Bezugly[2], Daria Kovalenko[3], Anna Czeschik[1], Richard Boucher[2], Jan Meiss[4], and Doru Lupascu[1] — [1]Institut für Materialwissenschaft, Universität Duisburg-Essen, Universitätsstrasse 15, 45141 Essen, Deutschland — [2]Institut für Werkstoffwissenschaft, Technische Universität Dresden, 01069 Dresden, Deutschland — [3]Fraunhofer-Institut für Zerstörungsfreie Prüfverfahren Institutsteil Dresden, IZFP-D, Deutschland — [4]Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Deutschland

In this study we focus on the dispersion of carbon nanotubes (CNT) and their characterisation using spectroscopic analysis. Single walled and multi walled carbon nanotubes (SWCNT, MWCNT) are used to form dispersions with different solvents. Besides surface-active agents we investigate a π-stacking approach to disperse the hydrophobic CNT. CNT bucky paper made by DNA-wrapped CNT dispersion include DNA. Covalent sidewall functionalisation of CNT to change their hydrophobic surface to a hydrophilic one will entail additional chains (commonly carboxylic chains) at the CNT sidewall due to the chemical treatment. If surface-active agents are used for preparation, a thoroughly rinsing after film preparation is necessary to remove agents. The π-stacking approach offers the advantage to evaporate all chemicals used for the dispersion via annealing and high purity is achieved. Therefore this technique could be a tool kit in organic semiconducting application.

CPP 38.30 Wed 17:00 P2

Hybrid method simulations of clay suspensions — •Hongliu Yang[1], Martin Hecht[2], and Heike Emmerich[1] — [1]Bayreuth University, Bayreuth, Germany — [2]High Performance Computing Center Stuttgart, Stuttgart, Germany

Clay colloids, in the form of suspensions of platelet particles, are the subject of an enormous recent studies. It is especially due to their widespread applications ranging from drilling, rheology modification for paints, cosmetics, cleansers, and the production of paper, adhesives, synthetic plastics etc. Clay colloid suspensions are different from other colloids by the high anisotropy of the dispersed thin crystalline silicate platelets. Moreover, faces and edges of clay particles may have different types of charges under pH value variation. These factors make the theoretical descriptions of clay suspensions very difficult. A hybrid code with molecular dynamics for clay particles and stochastic rotation dynamics for surrounding fluids is developed by us to simulate clay suspensions. In our simulations clay particles are modeled as charged soft ellipsoids interacting via Gay-Berne potential and screened Coulomb potential. The existence of analytical forms of the mutual interactions makes the calculation of force and torque very efficient. Preliminary results of micro-structures and rheological properties of clay suspensions are reported.

CPP 38.31 Wed 17:00 P2

Weight functions in fundamental measures density functional theory — •Markus Burgis and Matthias Schmidt — Theoretische Physik II, Physikalisches Institut, Universitätsstraße 30, D-95440 Bayreuth

An overview of the key geometrical ingredients of fundamental measures density functional theory is given. In particular the mathematical structure behind the four different types of scalar Kierlik-Rosinberg weight functions is investigated. These weight functions are used to represent the Mayer bond of hard sphere mixtures via pairwise convolution. The range of all weight functions, i.e. the hard sphere radius, can be changed by a convolution transformation. The relevance to both the fundamental measures density functional for additive hard spheres as well as to its generalization to non-additive binary mixtures is discussed.

CPP 38.32 Wed 17:00 P2

IPBS - An iterative Poisson Boltzmann Solver — •Alexander Schlaich — Institute for Computational Physics Universität Stuttgart Pfaffenwaldring 27 70569 Stuttgart

We present a finite element based method for solving the nonlinear Poisson Boltzmann equation in presence of dielectric missmatch with unknown boundary conditions. Such conditions apply for example to colloidal systems with counterions in solution where the field in the inner part of the particle is not of interest.

Proper boundary conditions are determined by an iterative, fast converging procedure which can be applied to arbitrary geometries. This algorithm allows us to solve a wide class of problems, for example in surface chemistry, colloidal science and general soft matter research, with high efficiency due to the reduced number of grid points. Calculation results are compared both to experimental data and theoretical predictions, e.g. those from DLVO theory.

CPP 38.33 Wed 17:00 P2

Entropy and enthalpy convergence of hydrophobic solvation beyond the hard-sphere limit — •Felix Sedlmeier, Dominik Horinek, and Roland Netz — Technical University Munich, Garching, Germany

The experimentally well-known convergence of solvation entropies and enthalpies of different small hydrophobic solutes at universal temperatures seems to indicate that hydrophobic solvation is dominated by universal water features and not so much by solute specifics. The reported convergence of the denaturing entropy of a group of different proteins at roughly the same temperature as hydrophobic solutes was consequently argued to indicate that the denaturing entropy of proteins is dominated by the hydrophobic effect. However, this appealing picture was subsequently questioned since the initially claimed universal convergence of denaturing entropies holds only for a small subset of proteins, for a larger data collection no convergence is seen. We report extensive simulation results for the solvation of small spherical solutes in explicit water with varying solute-water potentials. We show that convergence of solvation properties for solutes of different radii exists but that the convergence temperatures depend sensitively on the solute-water interaction. Accordingly, convergence of solvation properties is only expected for solutes of a homologous series that differ in the number of one species of subunits or solutes that are characterized by similar solute-water interaction potentials. In contrast, for peptides, it means that thermodynamic convergence at a universal temperature can not be expected in general, in agreement with experimental results.

CPP 38.34 Wed 17:00 P2

The Role of Charge Polarization in the Vibrational Dynamics of Ionic Liquids — •Mahdi Taghikhani and Oliver Kühn — Universität Rostock, Institut für Physik, Universitätsplatz 3, D-18051 Rostock

Different theoretical methods for describing the dynamics of the CH-stretching vibrations in imidazolium based ionic liquids ([C2min][NTf2]) are compared. This includes a description in terms of a classical molecular dynamics force field as well as hybrid quantum mechanics/molecular mechanics (QM/MM) approaches with a systematic variation of the partitioning into the QM and the MM parts. Special emphasis is put on the effect of charge polarization on the CH-stretching vibration which is part of a hydrogen bond linking two ions. Equipped with this information a strategy for efficient calculation of linear and nonlinear optical response functions is outlined which is based on the concept of transition frequency correlation functions.

CPP 38.35 Wed 17:00 P2

Bidisperse monolayers: what changes in 2D? — •Elena Minina[1], Alla Dobroserdova[1], Joan Cerda[2], Sofia Kantorovich[1,3], and Christian Holm[3] — [1]Ural State University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]Institute for Cross-Disciplinary Physics and Complex System, Campus Universitat de les Illes Balears, 07122, Palma de Mallorca — [3]Institute fuer Computerphysik, Universitaet Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Deutschland

Ferrofluid microstructure in the absence of an external magnetic field proves to be a function of two main parameters: ferroparticle density and intensity of the magnetic dipole-dipole interparticle interaction. It is also well known, that inherent polydispersity of ferroparticles makes the investigation of the structural transition in ferrofluids even more difficult. Earlier it was proposed to replace a continuous particle size distribution by a model bidisperse one [Ivanov et al, Phys. Rev. E, 2004]. The latter theoretical model provided a very good qualitative agreement on the ferrofluid microstructure with the simulation data [Holm et al, J. Phys: Condense Matter., 2006]. However, direct application of this approach to the description of ferrofluid monolayers (quasi-2D systems of ferroparticles [Klokkenburg et al., Phys. Rev. Lett., 2006]) failed and resulted in the regular qualitative discrepancies with the simulation data. In the present study we modify the free energy functional and show why the interplay of energy and entropy changes significantly ferrofluid microstructure in monolayers.

CPP 38.36 Wed 17:00 P2

Influence of an external magnetic field on a ferrofluid with chain aggregates — •Elena Pyanzina[1], Joan Cerda[2], Sofia Kantorovich[1,3], and Christian Holm[3] — [1]Ural State University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]Institute for Cross-Disciplinary Physics and Complex System, Campus Universitat de les Illes Balears, 07122, Palma de Mallorca — [3]Institute fuer Computerphysik, Universitaet Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Deutschland

We present the analysis of the influence of an external magnetic field on the ferrofluids with intensive interparticle magnetic dipole-dipole interaction. We investigate the structure factor of such systems by means of molecular dynamic simulations and theoretical modeling. In this study we focus on monodisperse systems, i.e. all particles are identical. The theoretical calculations are based on the explicit construction of radial distribution functions from the chain distributions in the presence of an external magnetic field obtained via density functional minimization. Molecular dynamic computer simulation are provided for the verification of the model and for elucidation of the connection between the scattering pattern and the system microstructure.

CPP 38.37 Wed 17:00 P2

Suspensions of particles with shifted magnetic dipoles — •Marco Klinkigt[1], Rudolf Weeber[1], Sofia Kantorovich[1,2], and Christian Holm[1] — [1]University of Stuttgart, Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgar — [2]Ural State University, Lenin av. 57, 620000, Ekaterinburg, Russia

In previous study we investigated the ground state for systems of particles, magnetic moment of which was shifted from the centre of mass, and pointed always outwards radially, using the combination of Monte Carlo simulations and analytical calculations. We showed that antiparallel orientation of moments becomes the most favorable ground state configuration when the shift approaches the particle radius. Our preliminary analysis of relatively small systems at room temperatures also showed a lot of interesting features. To study larger systems we used molecular dynamic simulation to reach better performance. Therefore, we implemented our model in ESPResSo, that allows us to use the P3M algorithm for dipolar long range interactions in systems with periodic boundary conditions in three dimensions. The also implemented MDLC gives us the possibility to simulate monolayers with periodic images in two dimensions. We obtained that the initial slope of the magnetization curves decreases with growing shift parameters. For higher magnetic interaction parameters we find initial slopes lower then the associated Langevin curve. Currently we are carrying out cluster analysis for the systems with different shifts and developing analytical expressions for magnetization laws.