CPP 16: Poster: Colloids and Complex Liquids

Time: Tuesday 18:15–20:45 Location: Poster A

CPP 16.1 Tue 18:15 Poster A

Directional locking of colloidal monolayers driven across quasiperiodic substrate potentials — •Thomas Bohlein and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Germany

Particles driven across an ordered potential energy surface may either follow the direction of the driving force or become entrained along any of the commensurate directions of the substrate. Such directional locking effects are of great technological relevance since they allow sorting of particles according to their size or refractive index. In recent numerical simulations it was predicted that kinetically locked-in states also occur on quasiperiodic potential landscapes which raises the question whether periodicity or long range order of the substrate is the essential ingredient for directional locking. Here we experimentally study the sliding behavior of a two dimensional colloidal monolayer interacting with quasiperiodic light induced substrate potentials. When the direction of the driving is varied with respect to the substrate, we find directional locking at angles corresponding to the symmetry axes of the underlying potential. On the locking steps the colloids exhibit a cooperative, kink-driven particle motion and assemble into dynamically ordered structures.

CPP 16.2 Tue 18:15 Poster A

Colloidal Epitaxy on Quasicrystalline Surfaces — •Sharan Devaiah, Thomas Bohlein, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Colloidal epitaxy is a powerful technique for creating three-dimensional structures useful for applications such as optical filters, switches and photonic materials. During this process, colloidal particles slowly sediment onto a patterned surface which then results in a highly ordered structure. Thus far, this process has only been used to create periodic colloidal crystals. Here, we report on experiments where we attempt to employ this process on templates with quasiperiodic order which are perfectly ordered but not periodic. Our experiments give us simultaneous access to the real space information and the diffraction pattern, thus enabling us to investigate if and how the initial quasiperiodic order of the template proliferates in the vertical direction through the monolayers.

CPP 16.3 Tue 18:15 Poster A

Phase behavior of colloidal monolayers on one-dimensional periodic and quasiperiodic light fields — •Lamiss Zaidouny and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Phase transitions of colloidal monolayers on light-induced substrate potentials have been demonstrated to provide novel insights into the phase behavior of two-dimensional systems on patterned surfaces. Due to the interplay of repulsive interparticle forces and their interaction with the substrate, interesting structures will form which are also observed in atomic systems. Here, we study the phase transitions of charged colloidal particles on arrays composed of one-dimensional laser lines which are created by a scanned laser beam whose diameter is highly asymmetric by passing a cylindrical lens. This allows the creation of laser lines with periodic and quasi-periodic order. In addition, to revisit light-induced freezing and melting, we present first results on how colloidal monolayers form in the presence of one-dimensional periodic potentials

CPP 16.4 Tue 18:15 Poster A

Colloidal flow and transport in micro structured porous media — •Frank Wirner[1,2], Christian Scholz[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany

The understanding of transport and flow phenomena in porous media is important for many problems which arise in various fields of science and engineering, ranging from agricultural, biomedical, chemical and petroleum engineering to soil sciences. Although the literature on porous media has been growing rapidly over the last decades it is still unclear, how transport properties of liquids through porous materials can be related to their structure. We study transport and flow properties of fluids and colloidal suspensions in a quasi-2D microporous system, created using soft lithography, over a wide range of flow regimes. The colloids act as tracer particles and visualize the flow field. A camera system with a temporal resolution of 2 ms and a spatial resolution of 0.4 μm is used to analyze the particle trajectories. The porous structures are artificially designed and therefore the structural parameters like Minkowski functionals and pore size distributions are fully known and can be related to dynamical flow variables, such as permeability or dispersion coefficients.

CPP 16.5 Tue 18:15 Poster A

Shape dependence of active Brownian particles — •Felix Kümmel — Universität Stuttgart, Stuttgart, Germany

We recently introduced a new species of active Brownian particles whose active motion is due to the local demixing of a critical binary liquid mixture and can be easily tuned by illumination [1]. Here, we focus on the shape dependence of such active swimmers, which are prepared by soft lithography. For chiral swimmers, we observe circular trajectories whose orientation depends on their chirality. When such particles come close to a straight wall, there are two different kinds of interaction. In one case, the particle slides stable along the wall, while in the other case it is reflected. In addition, other shapes of swimmers are investigated.

[1] G. Volpe, I. Buttinoni, D. Vogt, H.J. Kümmerer, and C. Bechinger. Microswimmers in patterned environments. Soft Matter, (7):8810{8815, 2011.

CPP 16.6 Tue 18:15 Poster A

Neutronscattering on discotic liquid crystals in the bulk and in the nanoconfined state — •Christina Krause[1], Bernhard Frick[2], Reiner Zorn[3], and Andreas Schönhals[1] — [1]BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — [2]Institut Laue-Langevin, 6 rue Jules Horowitz, BP. 156, 38042 Grenoble, France — [3]Research Centre Jülich, 52425 Juelich, Germany

Discotic liquid crystals (DLC) consist of a flat and rigid aromatic core substituted by flexible aliphatic chains. While the former is responsible for the pi-pi-stacking, the latter increases the solubility and gives rise to a rich thermotropic behavior. DLCs are self-assembled materials. The disc-shaped molecules organize into columns that further assemble into two-dimensional arrays with a hexagonal mesophase. The alkyl chains fill the intercolumnar space giving rise to a nanophase separated state. Triphenylene derivatives as model systems for DCLs were investigated by neutron scattering in the bulk and in the confined state where both the vibrational density of states as well as the molecular dynamics on a time scale of ca. 1 ns (elastic scans) were considered. The influence of both the structure (length of the aliphatic chains) and the confinement will be discussed in detail.

CPP 16.7 Tue 18:15 Poster A

Glassy dynamics in Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther studied by Differential Alternating Current Chip Calorimetry and Dielectric Relaxation spectroscopy — •Christina Krause, Huajie Yin, and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin

The glassy dynamics of the discotic liquid crystal Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther is investigated by a combination of Differential Alternating Current Chip Calorimetry and Dielectric Relaxation Spectroscopy. The temperature dependence of the dielectric relaxation rate in the low temperature range might be described by means of the Vogel-Fulcher-Tamann equation. A detailed analysis shows that the glassy dynamics changes in the vicinity of the phase transition temperature. To unravel a different aspect of the underlying processes Differential Alternating Current Chip Calorimetry is applied. Dielectric and calorimetric data show a good agreement. In the higher temperature limit charge transport is detected. Experiments on confined Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther are carried out in the near future.

CPP 16.8 Tue 18:15 Poster A

Block Copolymer Agglomerates in a Nematic Liquid Crystal — •Thomas Müller[1], Wolfgang Schöpf[1], Ingo Rehberg[1], Robin Pettau[2], Klaus Kreger[2], and Hans-Werner Schmidt[2] — [1]Experimental Physics V, University of Bayreuth, 95440 Bayreuth — [2]Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth

The suspension of colloidal particles in a nematic liquid crystal solvent can induce local disturbance of the director field. This effect is known from spherical particles like water droplets or gas bubbles which are injected into the liquid crystal host [1, 2]. We investigate a small amount of a side chain liquid crystal triblock copolymer in the nematic liquid crystal 5CB as solvent material. The middle block of the copolymer is 5CB-functionalized and therefore soluble in the anisotropic phase, whereas the non-soluble end blocks can aggregate due to microphase separation. If the resulting agglomerates are big enough, the director deformations in the surrounding birefringent area can be observed with a polarizing microscope. We study the optical properties of a thin layer of this side group liquid crystalline mixture between two glass plates and present a model for the director configuration around the agglomerates. [1] P. Poulin, D. A. Weitz, Phys. Rev. E, 57 (1), 1998; [2] C. Völtz, et al., Phys. Rev. Lett., 97, 227801, 2006

CPP 16.9 Tue 18:15 Poster A

Fluid-Fluid and Fluid-Solid transitions in the Kern-Frenkel model from Barker-Henderson thermodynamic perturbation theory — •Christoph Goegelein[1], Flavio Romano[2], Francesco Sciortino[3], and Achille Giacometti[4] — [1]MPI für Dynamik und Selbstorganisation, Goettingen — [2]Physical and Theoretical Chemistry Laboratory, Oxford University (UK) — [3]Dipartimento di Fisica and CNR-ISC, Sapienza Universita di Roma, Piazzale A. Moro 5, 00185 Roma, Italy — [4]Dipartimento di Scienze dei Materiali e Nanosistemi, Universita Ca' Foscari Venezia, Calle Larga S. Marta DD2137, I-30123 Venezia, Italy

We study the Kern-Frenkel model for patchy colloids using Barker-Henderson thermodynamic perturbation theory. The model describes a fluid where hard sphere particles are decorated with one patch, so that they interact via a square-well potential if they are sufficiently close one another, and if patches on each particle are properly aligned. Both the gas-liquid and fluid-solid phase coexistences are computed and contrasted against Monte-Carlo simulations results. We find that the perturbation theory describes rather accurately numerical simulations all the way from a fully covered square-well potential down to the Janus limit (half coverage). In the region where numerical data are not available (from Janus to hard-spheres), the method provides estimates of the location of the critical lines that could serve as a guideline for further efficient numerical work at these low coverages. A comparison with other techniques, such as integral equation theory, highlights the important aspect of this methodology in the present context.

CPP 16.10 Tue 18:15 Poster A

Dynamics in disconnected lamellar phases — •Stefan Wellert[1], Matthias Karg[2], Lukasz Szymanski[3], and Cosima Stubenrauch[3] — [1]TU Berlin, Str.d. 17.Juni 124, 10623 Berlin, Germany — [2]University of Bayreuth, Universitätsstrasse 30, 95440 Bayreuth, Germany — [3]University of Stuttgart, Pfaffenwaldring 35, 70569 Stuttgart, Germany

This contribution discusses the results of a neutron spin-echo (NSE) experiment addressing the dynamics in disconnected lamellar phases. (Pseudo)binary water-CiEj-type surfactant systems were investigated. The combination of a surfactant forming a continuous lamellar phase extending to low surfactant concentrations with a surfactant forming a lamellar phase only at high concentrations results in a disconnected lamellar phase. Regarding the stabilization of the lamellar phase in the dilute and the concentrated regime, respectively, it is known that the dilute lamellar phases, where the interlamellar distances are larger than the membrane thickness, are stabilized by membrane undulations. In the case of the concentrated lamellar phases, attractive van der Waals and repulsive steric forces are the stabilizing mechanisms. It was shown that the disconnection only takes place if the distance between two bilayers is similar to the thickness of the bilayers and it was argued that the disconnection is tuneable by the rigidity of the monolayer. In this combined small angle neutron scattering and NSE experiment we discuss the influence of the structure factor on the dynamics. By applying the theoretical approach of Zilman and Granek we determine the bending elasticity constants.

CPP 16.11 Tue 18:15 Poster A

Trapping colloids via critical Casimir forces — •Matthias Tröndle[1,2], Andrea Gambassi[3], Ludger Harnau[1,2], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — [2]Universität Stuttgart, Germany — [3]SISSA - International School for Advanced Studies and INFN, Trieste, Italy

Colloids opposite to substrates patterned with stripes of different chemical boundary conditions experience normal and lateral critical Casimir forces. Upon approaching the critical point of the solvent, this generates laterally confining potentials for the colloids. The strength of these trapping potentials is reversibly tunable by temperature changes. Experimental measurements for colloidal particles immersed in a binary liquid mixture of water and 2,6-lutidine close to the critical demixing point agree with the corresponding theoretical predictions [1,2]. It turns out that critical Casimir forces are a sensitive probe to the details of the geometry of the substrate pattern. A suitable choice of chemical stripes forming the pattern may even lead to *levitation* of colloids at a stable distance from the substrate due to the critical Casimir effect [3].

[1] M. Tröndle, O. Zvyagolskaya, A. Gambassi, D. Vogt, L. Harnau, C. Bechinger, and S. Dietrich, *Mol. Phys.* **109**, 1169 (2011). [2] M. Tröndle, S. Kondrat, A. Gambassi, L. Harnau, and S. Dietrich, *EPL* **88**, 40004 (2009). [4] M. Tröndle, S. Kondrat, A. Gambassi, L. Harnau, and S. Dietrich, *J. Chem. Phys.* **133**, 074702 (2010).

CPP 16.12 Tue 18:15 Poster A

Triphenylene-based discotic liquid crystals in bulk and confined to alumina oxide membranes — •Christina Krause, Huajie Yin, and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin

Discotic liquid crystals consist of a stiff aromatic core surrounded by flexible aliphatic side chains. As the disc-shaped molecules of the core self-organize into hexagonal columnar arrays, the alkyl chains fill the space between the columns yielding a nanophase separated state. A series of triphenylene-based discotic liquid crystals (2,3,6,7,10,11-Hexakis[n-oxy]triphenylene (HATn, n=5,6,8,10) is investigated by means of Dielectric Relaxation Spectroscopy, Differential Scanning and Differential Alternating Current Chip Calorimetry. Nanoporous alumina membranes with different pores sizes are filled with the triphenylene derivatives to study the influence of confinement on the dynamics in these discotic liquid crystals by means of Dielectric Relaxation Spectroscopy.

CPP 16.13 Tue 18:15 Poster A

Elastic Properties of nematic phase - DFT and simulations of hard spherocylinders — •Ellen Fischermeier, René Wittmann, and Klaus Mecke — Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

A fluid of hard spherocylinders is an ideal model system to study liquid crystals and to test density functional theories. Here we show results of a recent fundamental measure theory (FMT) generalized to arbitrarily shaped hard bodies [1]. This functional provides analytic expressions for the isotropic and nematic free energy as well as the Frank elastic coefficients of the nematic phase. However there is one free parameter in the functional which has to be adapted empirically. Therefore we carried out molecular dynamics simulations with a highly flexible and massively parallel rigid body framework [2]. The obtained numerical data is compared to the analytic results and we present the findings of both methods.

[1] H. Hansen-Goos and K. Mecke, Phys. Rev. Lett. **102**, 018302 (2009)
[2] Klaus Iglberger and Ulrich Rüde, Computer Science - Research and Development **23**, 159 (2009)

CPP 16.14 Tue 18:15 Poster A

Optical trapping of gold colloids — •Andreas Königer and Werner Köhler — Physikalisches Institut, Universität Bayreuth

Using a strongly focused laser beam to trap and manipulate single colloidal particles is a well known procedure in life science and micro rheology. We have extended this technique using a convergent laser beam, with its focus well above a thin sample layer, to be able to manipulate many colloids simultaneously. Operating with an inverted microscope we have shown, how sedimented gold colloids can be lifted against gravity and collected in an almost 2-dimensional cage by radiation forces that act against the osmotic pressure of the compressed colloidal gas. Once collected, the cloud of colloids can be manipulated in a number of

ways. It can freely be moved to arbitrary positions, where e.g. specific chemical reactions could take place. By time-multiplexing of the laser beam it is even possible to split the cloud into subensembles, which can than be manipulated independently and later be recombined by contact free purely optical means. We present a detailed analysis of the particle dynamics in the convergent light field and compare it to experimental data.

CPP 16.15 Tue 18:15 Poster A

Transient cage forming in polymer solutions by hot gold colloids — •Florian Schwaiger and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Germany

Utilizing laser heated gold colloids with a radius of 125 nm as nanoscopic heat sources, we investigated the concentration bleaching in binary polymer solutions of polystyrene and toluene due to the Soret effect. Laser irradiation causes a significant temperature rise $T \propto 1/r$ due to the high absorbance at their surface plasmon resonance around 532 nm. As a consequence of the strong nonlinear coupling of the local order parameter to the temperature gradient, it induces a complex concentration field $c(t, r, M_w, T(r))$. We analyze in detail the stationary temperature, concentration and viscosity profiles. Furthermore, we present experimental results both on the observation of the concentration field and on the diffusion of heated colloids within their self-created cage. We find increasing anomalous diffusion with increasing laser power represented by a negative minimum in the step correlation function of the random walk.

CPP 16.16 Tue 18:15 Poster A

Spontaneous emulsification of thermotropic liquid crystals in aqueous surfactant solutions — •Karthik Peddireddy, Pramoda Kumar, Shashi Thutupalli, Stephan Herminghaus, and Christian Bahr — Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Thermotropic liquid crystals (LCs) are organic liquids which are usually not miscible with aqueous phases. The presence of surfactants enables the generation of LC-in-water and water-in-LC emulsions, provided that sufficient mechanical energy is added to the system; in that respect the LC/water systems behave just as numerous non-LC oil/water systems.

We have recently observed that some common LC compounds (such as, e. g., the 4-n-alkyl-4′-cyanobiphenyls) can undergo a *spontaneous* emulsification process, running without addition of mechanical energy, when brought in contact with aqueous surfactant solutions. The details of the process and the observed transient structures depend on the type of the LC phase: For nematic phases we observe the formation of aqueous droplets in the nematic bulk phase as well as nematic droplets in the aqueous bulk phase. For smectic phases, transient structures appear which resemble the myelin figures formed by lyotropic lamellar phases in contact with water. Polarizing microscopy and fluorescence microscopy studies are conducted in order to elucidate the mechanism of this possibly new type of spontaneous emulsification.

CPP 16.17 Tue 18:15 Poster A

Friction within single pairs of DNA grafted colloids as studied by optical tweezers — •Mahdy M. Elmahdy[1,2], Olaf Ueberschär[1], Carolin Wagner[1], Tim Stangner[1], Christof Gutsche[1], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, Germany — [2]Department of Physics, Mansoura University, Mansoura 35516, Egypt

Optical Tweezers are employed to study the transition from sliding to stick-slip friction between two DNA grafted (grafting density ~1000 molecules per particle, number of base pairs per grafted chain ~4000) colloids. The latter are moved with a relative velocity in respect to each other ranging between 50 nm/s up to 3 μm/s; one colloid is fixed to a micropipette while the other is held in the optical trap hence enabling one to determine and to separate the forces of interaction in the direction parallel and perpendicular to the motion. Further parameter to be varied is the salt (NaCl) concentration of the surrounding medium at pH 8.5. A transition from sliding to stick-slip friction is found and shown to be controlled by the product of interaction volume and interaction time.

CPP 16.18 Tue 18:15 Poster A

Investigation of confinenment induced oscillatory forces in nanoparticle-suspensions by CP-AFM — •Sebastian Schön, Yan Zeng, and Regine von Klitzing — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Strasse des 17.Juni 124, D-10623 Berlin

Thin films of nanoparticles suspensions show a layered ordering in the vicinity of the confining surfaces, giving rise to oscillatory changes in density and force. These originate from the entropic excluded volume effect and indicate a break in the translational symmetry of the bulk system. The study of oscillatory forces therefore serves as a direct means to understand the interactions between colloids and control their stability.

Force measurements have been performed by Colloidal Probe Atomic Force Microscopy (CP-AFM), where the colloidal probe on the cantilever and the substrate act as confining surfaces. Forces can be extracted form the deflection signal of the cantilever and are normalized with the radius of the colloidal probe.

In previous investigations the influence of particles concentration, size and ionic strength of the suspensions has been studied. Using Small Angle X-Ray Scattering (SAXS) good agreement of the characteristic lengths between confinement and bulk was demonstrated.

Latest research focus on effect of surface potential of the nanoparticles on the oscillatory forces investigating different systems of silica nanoparticles and micelles.

CPP 16.19 Tue 18:15 Poster A

Critical Casimir torques acting on cylindrical colloids and Janus particles — •Marcel Labbé-Laurent[1,2], Matthias Tröndle[1,2], Ludger Harnau[1,2], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für intelligente Systeme, Stuttgart, Germany — [2]Universität Stuttgart, Germany

Critical fluctuations in fluids give rise to forces acting on immersed colloidal particles. These Casimir-like forces are attractive or repulsive depending on the chemical surface properties. Self-assembly of colloids opposite to *structured* surfaces, induced by the critical Casimir effect, is observed experimentally for colloidal particles immersed in a critical water-2,6-lutidine mixture and is in agreement with theory [1]. Asymmetrical particles experience a critical Casimir torque in the presence of varying boundary conditions. The strength and the direction of the torque depend on the particle shape. Rod-like and disc-like particles exhibit different self-orientation. Similarly, *Janus*-particles are subject to critical Casimir torques and self-orientate, which may be useful in view of current research or applications.

[1] M. Tröndle, O. Zvyagolskaya, A. Gambassi, D. Vogt, L. Harnau, C. Bechinger, and S. Dietrich, *Mol. Phys.* **109**, 1169 (2011).

CPP 16.20 Tue 18:15 Poster A

Confocal Microscopy of Colloidal Hard Sphere and Charged Sphere Fluids and Crystals — •Achim Lederer and Hans Joachim Schöpe — Johannes Gutenberg University, Mainz, Germany

Monodisperse suspensions of colloidal spheres with known interaction are a terrific model system for testing predictions by statistical physics. Their typical length scales are accessible via optical methods like light scattering in reciprocal and microscopy in real space. Light scattering leads to ensemble averaged observables like structure factors in reciprocal space with a high statistical accuracy, while information about the local order and the local dynamic are very difficult to get. A state-of-the-art technique to gain information about the local parameters of a colloidal system is the Laser Scanning Confocal Microscope (LSCM) which takes 3D-videos from a sample. By this method, the structure and dynamics of a colloidal suspension can be observed on a single particle scale ([1], [2]). In this work we investigate colloidal model systems with hard sphere and charged sphere interaction in the fluid and crystalline regime using LSCM. We determine the structure of the colloidal fluid in the equilibrium state as well as in the metastable regime showing significant differences between these states increasing with increasing metastability.

[1] V. Prasad et al., J. Phys.: Condens. Matter 19, 113102 (2007).
[2] A. D. Dinsmore et al., Appl. Opt. 40, 4152 (2001)

CPP 16.21 Tue 18:15 Poster A

Magneto-optical Technique for Detecting the Biaxial Nematic Liquid Crystal Phase — •Tanya Ostapenko[1], Cuiyu Zhang[2], Samuel Sprunt[1], Antal Jákli[2], and James Gleeson[1] — [1]Department of Physics, Kent State University, Kent, Ohio 44242, USA — [2]Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, Kent, Ohio 44242, USA

The existence of the biaxial nematic liquid crystal phase (N_b) has been the subject of much discussion since it was first predicted [1]. The ge-

ometry of the liquid crystal mesogen is important and it is thought that banana-shaped, or bent-core, liquid crystals will have an N_b phase. Recently, there have been attempts to find a bent-core liquid crystal that exhibits this phase, but there have been many conflicting reports about whether the N_b phase has been positively identified. One reason for the discrepancy is that there is currently no way to rule out surface effects or anchoring transitions, both of which may give a false positive identification of a uniaxial-biaxial nematic transition. Optical techniques usually rely on a sample cell rubbing treatment to align the sample, but optical misidentification could occur if the material is in a tilted uniaxial phase, which appears the same as a homeotropically-aligned biaxial phase. We have developed a technique that uses a magnetic field to align the uniaxial director, thus widening its application to any bent-core nematic material.

[1] M.J. Freiser. *Phys. Rev. Lett.* **24**, 19, 1041-1043 (1970).

CPP 16.22 Tue 18:15 Poster A

Dynamic percolation in microemulsions based on anionic and nonionic surfactants — •Andreas Bischof, Christina Lederle, Andreas Weber, Tinka Spehr, and Bernd Stühn — TU Darmstadt, Experimentelle Physik kondensierter Materie, Germany

We study structure and dynamics of water-in-oil microemulsions with a focus on dynamics percolation phenomenon. In order to do this, we use dielectric spectroscopy. Comparing microemulsions based on different surfactants, we see a significant change in the percolation behaviour. We compare water-in-oil microemulsions based on anionic (AOT: Dioctyl sodium sulfosuccinate) and nonionic (i.e. C12E4: Pentaethylene glycol monododecyl ether) surfactants. Both display the known phenomenon of percolation that manifests itself in a steep increase of conductivity changing composition or temperature. We focus on the droplet phase and the temperature dependent behaviour to estimate the percolation temperature Tp. The percolation transition is observed with increasing temperature for ionic surfactants and decreasing temperature for nonionic surfactants. Moreover in the case of nonionic surfactant based microemulsions we study the effect of addition of salts. We compare results from dielectric spectroscopy to structural findings by means of small angle x-ray scattering (SAXS).

CPP 16.23 Tue 18:15 Poster A

Interactions between PEG and non-ionic surfactant layers — •Andreas Weber, Andreas Barz, Tinka Spehr, and Bernd Stühn — Experimentelle Physik kondensierter Materie, Technische Universität Darmstadt

The interactions between polymers and soft surfactant layers are subject of current research interest. One system to study these interactions are microemulsions, thermodynamic stable mixtures of a polar liquid and a non-polar liquid stabilized by a surfactant. Depending on the composition of the system, these microemulsions can form various structures. One of these structures is the droplet phase. There, droplets of one component are dispersed in a matrix of the other component. We examine the phase diagrams of water in oil droplets stabilized by a non-ionic surfactant ($C_{12}E_5$, $C_{12}E_4$) to characterize the initial system by small angle X-ray-scattering and light transmission experiments. We add the hydrophilic polymer PEG to the microemulsion to investigate the interactions between these polymers and the curved surfactant layer of the droplets: While scattering experiments provide information about the structure of the interface, dynamic light scattering and dielectric spectroscopy give results concerning the dynamics of the droplets and the interface. Furthermore, by changing temperature it is possible to force the initial system into a lamellar phase. We also examine the effect of adding polymer to those structures.

CPP 16.24 Tue 18:15 Poster A

Ferrocene-Pyridine Block Copolymers in Solution - Cylindrical Micelles in Methanol — •Stephan Hillmann[1], Martin Kraska[1], Markus Gallei[2], Roland Klein[2], Matthias Rehahn[2], and Bernd Stühn[1] — [1]Experimentelle Physik kondensierter Materie, TU Darmstadt — [2]Ernst-Berl-Institut für Technische und Makromolekulare Chemie, TU Darmstadt

Ferrocene-containing polymers attract much attention because of their unique mechanical, (electro)chemical, (opto)electronical or magnetic properties [1]. We present structural investigations of the block copolymer poly(vinylferrocene-b-(2-vinylpyridine)) (PVFc-b-P2VP) [2] dissolved in methanol. Results from Small angle X-Ray scattering (SAXS) and polarized and depolarized dynamic light scattering (DLS) are combined leading to a detailed understanding of the structure in solution [3]. We found cylindrical micellar structures with different length to diameter ratios depending on the bulk volume fraction ϕ of PVFc in P2VP. Cylindrical diameters could be determined by DLS and SAXS. We applied different diffusion models to the DLS data in order to extract cylinder lengths and diameters. Both scattering methods support the image of a solution of isolated dissolved cylinders.

[1] G. R. Whittell, I. Manners, Adv. Mater. 2007, 19, 3439
[2] M. Gallei et al. Macromolecules, 2010, 43 (4), 1844-1854
[3] M. Kraska, S. Hillmann, M. Gallei, R. Klein, M. Rehahn, B. Stühn, *in preparation*

CPP 16.25 Tue 18:15 Poster A

Predicting the Soret coefficient in binary mixtures via an additiv model of the heats of transport — •Florian Schock, Steffen Hartmann, and Werner Köhler — Physikalisches Institut, Universität Bayreuth

Diffusion in a binary mixture not only originates from a concentration but also from a temperature gradient. The so-called Soret coefficient, which is the ratio of thermal diffusion coefficient and mutual mass diffusion coefficient, can be expressed by non-equilibrium quantities - the heats of transport -, and a thermodynamic factor that can be obtained from equilibrium properties. We have measured the Soret coefficient of a large number of binary mixtures of organic solvents at least at three different concentrations. The thermodynamic factors have been determined from the group contribution method Modified UNIFAC (Dortmund). We have found an additive model for the heats of transport of equimolar mixtures. This allows to predict the Soret coefficients of all possible symmetric binary mixtures from the measurement of a single system. The procedure is exemplified for a series of alkanes in comparison with existing data for a large number of solvents.

CPP 16.26 Tue 18:15 Poster A

Rotational behavior of thermophoretic driven Janus particles at a hard wall. — •Andreas Bregulla[1], Ralf Seidel[2], Michael Mertig[3], Klaus Kroy[4], and Frank Chichos[1] — [1]Molecular Nanophotonics Group, University Leipzig — [2]DNA Motors Group, University of Technology Dresden — [3]Physikalische Chemie, Technische Universität Dresden — [4]Soft Condensed Matter Theory Group, University Leipzig

Janus particles are particles with asymmetric surface properties of their two half spheres. Due to this asymmetry they become of large interest as building blocks for new self-organized structures or they provide new unique optical properties if one site of the sphere is coated by noble metal films. In the latter case of a metallic coating of one half, the metal can be used as optically driven heat source to generate an asymmetric temperature distribution around the particle. This asymmetric temperature distribution leads to a thermophoretically driven directed motion of the particle as recently demonstrated. The detailed mechanisms of this driven motion is,however, not clear. Especially the contributions of local charge distributions, field enhancements and the interaction with substrate is unknown. In this contribution we investigate the rotational motion of gold capped polystyrene spheres nears a boundary with help of darkfield imaging and demonstrate that the interaction with the surface leads to a restricted rotational motion.

CPP 16.27 Tue 18:15 Poster A

An ionic liquid electrospray source based on the epoxy SU-8 — •Katharina Huhn, Markus Piechotka, Torsten Henning, and Peter J Klar — I. Physikalisches Institut, JLU Gießen

In this work the feasibility of SU-8 capillaries for the application in an electrospray source was investigated. The interaction between the capillaries and the applied ionic liquids was examined in detail. Therefore we manufactured a test system consisting of three patterned layers: two layers of SU-8 as well as a metallic extraction electrode. The SU-8 layers were structured by means of photolithography whereas the extraction grid was grown by electroplating. The ionic liquid droplet formation was observed by micrograph imaging. Furthermore the influence of an electric potential between extraction electrode and ionic liquid was investigated.

CPP 16.28 Tue 18:15 Poster A

Comparison of time-dependent friction and diffusion coefficients of single blank and DNA-grafted colloids in dilute polymer solutions - Drag reduction by DNA-grafting beyond linear response? — •Olaf Ueberschär, Carolin Wagner, Tim Stangner, Christof Gutsche, and Friedrich Kremer — Institut für Experimentelle Physik I, Universität Leipzig

Recently, we discovered that single DNA-grafted colloids under shear flow in dilute λ-DNA solutions experience a drag force that is significantly reduced compared to equally sized blank microspheres. The maximum extent of this drag reduction was found to amount to 60% compared to the λ-DNA-induced contribution on the drag on blank colloids. Based on previous theoretical work, we proposed an explanation of this effect by analyzing the differences in the Stokes flow field around the blank and grafted colloids. Now, we present new experimental and theoretical results that help to elucidate further the effects of polymer accumulation and depletion around single colloids in dilute polymer solutions under thermal equilibrium and non-equilibrium steady state conditions. Special emphasis is laid on the question whether or not these effects still take place in the linear response regime. For this, we compare the experimental data obtained with our optical tweezers setup and a fast free particle tracking measurements. The two major measurement approaches towards friction coefficients on a single particle level (drag forces in Stokes flow, free diffusion paths) are discussed in detail. Good quantitative agreement with pertinent theoretical predictions further supports our argumentation and conclusions.

CPP 16.29 Tue 18:15 Poster A

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

In two-dimensional systems topological defects always occur as dislocation, pairs of dislocation or disclinations. These defects appear already near kbT and distort the hexagonal symmetric of the 2D crystal, whereby, according to the Kosterlitz-Thouless-Halperin-Nelson-Young theory, melting in 2D proceed. On the other hand so called geometric defects as isolated point defects need a lot more energy to be created which can experimentally be done with an optical tweezer. We study the particle configurations and the displacement fields of several defects in a 2D system of paramagnetic colloidal particles which are sediment to a water/air-interface. By applying a magnetic field perpendicular to the interface 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 and their interaction. Furthermore we study the formation of defect strings by creating more than two defects of the same kind, which rearrange and form a string consisting of two dislocations and a number of vacancies or interstitials in between.

CPP 16.30 Tue 18:15 Poster A

Microrheology using Optical Tweezers — •Christof Gutsche, Olaf Ueberschär, Carolin Wagner, Tim Stangner, and Friedrich Kremer — Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, Germany;

Optical Tweezers are ideal tools to carry out microfluidic and microrheological experiments with micrometer-sized objects. They enable one to measure without any mechanical contact forces acting on a particle with the extraordinary resolution of up to 5 fN. Experiments are presented on (i) the flow resistance of single DNA-grafted colloids in different media [1,2], (ii) the flow resistance of one blank colloid in a polymer solution [3] and (iii) the effective hydrodynamic radius of single DNA-grafted colloids as measured by fast Brownian motion analysis [5].

[1] C. Gutsche, M. Salomo, Y.W. Kim, R.R. Netz and F. Kremer. Microfluidic Nanofluidic 2(5), 381 (2006) ; [2] Y.W. Kim, V. Lobaskin, C. Gutsche, F. Kremer, P. Pincus and R.R. Netz. Macromolecules 42, 3650 (2009); [3] C. Gutsche and F. Kremer, M. Krueger and M. Rauscher, R. Weeber and J. Harting. J. Chem. Phys. 129, 084902 (2008); [4] C. Gutsche et al. Phys. Rev. E 76, 031403 (2007); [5] O. Ueberschär et al. Polymer 52, 1829 (2011)

CPP 16.31 Tue 18:15 Poster A

Microfabrication of a 3D asymmetric flow profile for chiral separations — •Carina Vossköttter, Lukas Bogunovic, and Dario Anselmetti — Experimental Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld University, Bielefeld, Germany

Chiral molecules (enantiomers) are molecules with the same molecular formula that can be transformed into the respective other isomer only by mirroring. Even if enantiomers - except for their optical activity - yield identical physical properties, they can still have completely different biochemical effects with respect to the metabolism of living organisms. At the present time, industrially synthesized chiral drugs are separated as far as required so that 25 % of all them are administered as pure enantiomers.

We conceived an alternative selector-free and continuously working concept to separate chiral objects within a lab-on-a-chip device. We show that it is possible to separate (asymmetric) chiral micro-objects within an asymmetric micro flow profile with a yield of 85 %.

Furthermore this so far two-dimensional concept is expanded into full 3D by introducing a novel two-component assembly strategy for the microchip, that can allow for a complex surface modification protocol to break the symmetry in every relevant dimension.

CPP 16.32 Tue 18:15 Poster A

Electron spectroscopy study of the interaction of copper with [EMIm]Tf_2N under the influence of aerobic conditions — •André Zühlsdorff, Angela Ulbrich, Markus Reinmöller, Wichard J. D. Beenken, and Stefan Krischok — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany

The interest of Cu/Ionic Liquid (IL) systems is motivated by the possibility to produce Cu nanoparticles as well as the great potential for catalytic processes. A detailed knowledge of the electronic structure of the Cu/IL system and the behaviour under environmental conditions is therefore important. Due to the low vapour pressure of ILs it is possible to analyse their properties under ultra high vacuum (UHV) conditions. In the present study copper was deposited onto [EMIm]Tf_2N by electron beam evaporation. Afterwards the influence of copper on the surface electronic structure of [EMIm]Tf_2N was investigated by X-ray photoelectron spectroscopy (XPS). An enrichment of copper at the edge of the liquid film was observed. The storage of the Cu/IL system under aerobic conditions for several days leads to a formation of Cu^{2+} species. Additionally, a modification of the near surface chemical composition was found and will be discussed. By comparing the copper containing IL with the neat [EMIm]Tf_2N a modification of the valence band structure was observed. The reconstruction of the photoelectron spectra by density functional theory (DFT) gives decent hints to the origin of these additional valence band structures.

CPP 16.33 Tue 18:15 Poster A

Efficiency boosting in application: Influence of the Poloxamer size on the phase behaviour of skin friendly microemulsions for decontamination — •Sebastian Höhn[1], Ralph Neubauer[1], Christoph Schulreich[1], André Richardt[2], and Thomas Hellweg[1] — [1]Phys. und Biophys. Chemie (PC III), Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]WIS Munster, ABC-Schutz, Humboldtstraße 100, 29633 Munster, Germany

Bicontinuous microemulsions exhibit sponge-like domain structures of oil and water separated by an enormous surfactant interface and are therefore excellent media for enzymatically catalysed reactions.

The addition of small portions of amphiphilic polymers can increase the efficiency of the surfactant, a phenomina known as the efficiency boosting effect. In this contribution the influence of the size of different commercially available triblock copolymers (Poloxamers) on two systems composed of sugar surfactant, alcohol, water, and oil is shown.

With the added block copolymers being a part of the amphiphilic interface, their effect on the size of the domains is of high interest. The results of small angle scattering methods (SAXS and SANS) for our model system based on n-decyl-β-D-maltoside ($C_{10}G_2$) and cyclohexane are compared with a technical system consisting of Simulsol SL55 ($C_{10-12}G_{1.3}$, Seppic) and Lanol99 (isononyl-isononate, Seppic). Here the influence of different Pluronic Polymers (BASF) on the phase diagram is presented.

CPP 16.34 Tue 18:15 Poster A

Analyzing polydispersity and deformation in confocal images of colloids — M. Roth, J. Wenzl, M. Franzmann, and •G. K. Auernhammer — MPI Polymer Research, Mainz, Germany

Confocal microscopy has been used to study the dynamical and structural properties of colloidal and granular matter. Three dimensional positions and translational motions of the constituent particles can be measured with high precision. Other quantities like forces or rotational motions, or the analysis of polydisperse samples, are harder to address.

Forces between particles in contact lead to deformations of the particles. For soft hollow spheres these deformations are large enough to be identified from confocal images. We present an extension to the algorithm by Crocker and Grier [1] to automatically extract the deformation particles (absoltute values and orientation) and thus forces on the particle. For this we use colloids that are only labelled in their

surface. Convoluting the image of deformed hollow spheres with the expected image of the undeformed state leads to a correlation peak that carries the information about the deformation [2].

Additionally we show how to detect reliably the coordinates of polydisperse colloids in confocal images. We develop methods to reliable measure the position and extension of spherical particles. To illustrate the applicability of this algorithm we show the restructuring of colloidal aggregates under mechanical stress.

[1] J. C. Crocker and D. G. Grier, J. Coll. Int. Sci., **179**, 298 (1996).

[2] M. Roth, M. Franzmann, M. D'Acunzi, M. Kreiter, and G. K. Auernhammer, arXiv:1106.3623v1 [cond-mat.soft] (2011).

CPP 16.35 Tue 18:15 Poster A

Structure factor of model polydisperse ferrofluids with relatively weak interparticle interactions — •Ekaterina Krutikova[1], Sofia Kantorovich[1,2], and Alexey Ivanov[1] — [1]Ural Federal University, Lenin av 51, 620083, Ekaterinburg, Russia — [2]Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart

Scattering measurements allow to obtain the so-called structure factor, which is, actually, the Fourier transform of the pair correlation function of the ferroparticle system. Thus, for correct processing of experimental data it is necessary to develop the theoretical model for the pair correlation function and structure factor. Here, we present a theory based on the diagram expansion of the pair particle potential, and molecular dynamics simulations for various polydisperse systems, and analyse the behaviour of the first peak of the structure factor, namely its height and width as a function of the ferrofluid granulometric composition.

CPP 16.36 Tue 18:15 Poster A

Magnetic properties of ferrofluids with shifted dipoles — •Taisia Prokopieva[1] and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av 51, 620083, Ekaterinburg, Russia — [2]Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart, Germany

A statistical model has been developed to describe the magnetic properties of ferrofluids with shifted dipoles. Using the model, which is based on the "mean-field approach" [Ivanov A., Kuznetsova O., Physical Review E, 2001], we calculate the magnetization and initial susceptibility of the system of particles in which the dipole moment is shifted out from the center of mass towards the particle surface. Magnetic characteristics are calculated in the form of an expansion over the special potential of the interparticle interaction for shifted dipoles [Kantorovich S., Weeber R., Cerda J., Holm Ch., Soft Matter, 2011]. The influence of the relative shift of the magnetic moment (that is the ratio of the shift to the radius of the particle) on the magnetic properties of the system is demonstrated.

CPP 16.37 Tue 18:15 Poster A

Effective Confinement as Origin of the Equivalence of Kinetic Temperature and Fluctuation-Dissipation Ratio in a Dense Shear Driven Suspension — •Boris Lander[1], Udo Seifert[1], and Thomas Speck[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Germany — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Germany

In equilibrium, the fluctuation-dissipation theorem states that the ratio of a correlation function and the corresponding response function is time independent, its value - the fluctuation dissipation ratio (FDR) - is given by the thermal energy. Out of equilibrium, this time independence is not expected to hold anymore. However, studying response and velocity autocorrelation functions for a tagged particle in a shear driven colloidal suspension, we found a broad regime where this time independence still holds approximately to a very good degree. The approximately constant FDR is the kinetic temperature. We can now explain this a priori surprising observation, using the idea of an effective confinement in dense suspensions [1]. Exploiting a time-scale separation, we can derive an approximate form of the FDT involving the kinetic temperature as a constant scaling factor and an additive correction term. We show numerically that the latter is negligible in a broad parameter range. We also compare the system to a simple toy model, consisting of a single colloidal particle, trapped in a harmonic potential, subjected to shear flow. For this simple model, we also find a regime in which the FDR is approximately time-independent.

[1] B. Lander, U. Seifert, and T. Speck arXiv:1111.3589

CPP 16.38 Tue 18:15 Poster A

Non-equilibrium simulations of confined colloidal particles — •Tarlan Vezirov and Sabine H. L. Klapp — Institute of Theoretical Physics, Secr. EW 7-1, Technical University Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

We consider a confined non-equilibrium system of interacting colloidal particles driven by a planar shear flow. As a framework for solving the equation of motion,we employ the Molecular and Brownian Dynamics simulations. We investigate the impact of the shear flow and confinement on transport properties such as density profiles, mean-squared displacements and the diffusion coefficient.

CPP 16.39 Tue 18:15 Poster A

Time Dependent Excited State Solvation of a Polarity Probe — •Christoph Allolio and Daniel Sebastiani — Freie Universität Berlin Fachbereich Physik Arnimallee 14 14195 Berlin

The molecular probe *N*-methyl-6-quinolone (MQ) gives spectroscopic access to its local environment.[1] Using *ab-initio* molecular dynamics, we have simulated the excited state solvation of MQ[2] and the time evolution of its Stokes shift in aqueous solution. Results are in good agreement with experimental data obtained using femtosecond spectroscopy. The effect of electronic excitation is discussed in terms of the actual atomistic coupling to the surrounding hydrogen bond network and dipolar relaxation. Our understanding of the time dependent aqueous solvation around MQ is then used to investigate hydrogen bonding dynamics in complex biophysical systems available to experimentalists.[3]

1 Pérez-Lustres, J. L., Mosquera, M., Senyushkina, T., Kovalenko, S. A., Flasche, W., Ernsting, N. P. Angew. Chem. Int. Ed., 44, 5635-5639. (**2005**)

2 C. Allolio and D. Sebastiani, Phys. Chem. Chem. Phys., 13, 16395-16403. (**2011**)

3 Sajadi, M., Ajaj, Y., Ioffe, I., Weingärtner, H., Ernsting, N. P. Angew. Chem. Int. Ed., 49, 454-457. (**2010**)

CPP 16.40 Tue 18:15 Poster A

Percolation transition of colloids in confined geometry — •Helge Neitsch and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We have performed grand canonical Monte-Carlo simulations to investigate the percolation transition of a system consisting of colloidal particles in the bulk as well as in a slit pore system, where the particles are confined by two plain, smooth and parallel walls. The colloidal interaction is simply modeled via a square well potential with a short range of attraction of 4% of the hard core diameter. The percolation transition is linked to interesting physical properties like colloidal gelation, conductivity or the connectivity of cavities within porous media. In agreement with a recent publication [1] our results lead to the finding, that the critical exponents of the bulk and of the confined system are deviating from those of the 2D or 3D random percolation class. We furthermore present results for the influence of the wall separation on the locus of the percolation threshold [paper in preparation].

[1] J. Skvor and I. Nezbeda, Mol. Phys. **109**, 133-139 (2011)

CPP 16.41 Tue 18:15 Poster A

On a field-induced vapor-liquid phase transition in dipolar monolayers — •Sebastian Jäger, Heiko Schmidle, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate suspensions of colloidal dipolar particles in quasi-two-dimensional systems that are exposed to external rotating fields. If the fields rotate within the plane of the dipolar monolayer and are of suitable strength and frequency [1], they can cause the particles to self-assemble into two dimensional aggregates. In this talk, we relate the cluster aggregation process to a vapor-liquid phase transition and investigate the dynamic behavior of the dipolar particles when exposed to the rotating fields. To do this, we make use of Brownian (Langevin) dynamics simulations (with and without hydrodynamic interactions) and Monte-Carlo simulations [2, 3].

[1] S. Jäger and S. H. L. Klapp, Soft Matter 7, 6606 (2011).

[2] H. Schmidle and S. H. L. Klapp, J. Chem. Phys. 134, 114903 (2011).

[3] S. Jäger, H. Schmidle, and S. H. L. Klapp, in preparation.

CPP 16.42 Tue 18:15 Poster A

Colloidal crystals confined by walls: static and dynamic aspects of structural transitions caused by misfit — •Dorothea

Wilms, Peter Virnau, and Kurt Binder — Johannes Gutenberg Universität, Mainz

A two-dimensional colloidal crystal is studied under confinement of structured walls in one direction. Introducing a misfit by placing the walls closer together leads to a structural transition from n rows to (n-1) rows of crystalline particles and the development of soliton-staircases.

This system is investigated using Langevin Dynamics. We discovered an unusual mechanism of diffusion, where groups of particles make a collective circular movement.

The same system has been investigated under shear. Depending on the shear velocity, different effects were observed, ranging from the development of holes in the system to large parts of the crystal changing the orientation of their layers.

CPP 16.43 Tue 18:15 Poster A

Phase behavior of microemulsions with weak and strong surfactants — Harsha Paroor and •Doris Vollmer — MPI for Polymer Research, Mainz, Germany

Microemulsions are thermodynamically stable, isotropic mixtures of water, oil and surfactant. Depending on the temperature and concentration, surfactant molecules associate into a micellar, lamellar, hexagonal or sponge like bicontinous structure. To quantitatively predict the phase behavior we proposed a modified Helfrich equation describing the morphologies. It assumes that within a well-defined temperature interval two spontaneous curvatures coexist. To investigate the validity of this assumption we investigate the phase boundaries by various measurements. The spontaneous curvature is calculated from fitting the emulsification boundaries. Experimentally determined values for the phase transition temperatures and specific heat have been successfully fitted to the unified model.

CPP 16.44 Tue 18:15 Poster A

Disentangling Free-Energy and Diffusivity Contributions of Water Kinetics in Bulk and at Interfaces — •Yann von Hansen[1,2], Felix Sedlmeier[1], Liang Mengyu[1], Dominik Horinek[1], and Roland R. Netz[1,2] — [1]Physik Department, TU München — [2]Fachbereich Physik, FU Berlin

We use a recently developed method based on the Fokker-Planck equation [1] to disentangle the contributions of the free energy and diffusivity profiles on the local stochastic dynamics of single water molecules in bulk and at interfaces. Based on the trajectories of the separation between water molecule pairs from MD simulations, we investigate the bond breakage dynamics in bulk water. From the spectrum of mean first-passage times, the diffusivity profile along the separation coordinate is derived. The six-fold friction increase at small separations and the variations in the diffusivity profiles can be interpreted in terms of a dominant reaction path that involves additional orthogonal coordinates [2]. Using the same methodoly, we study the water kinetics at hydrophobic and hydrophilic substrates and solutes and obtain diffusivity profiles showing significant differences, which can be attributed to the presence of hydrogen bonds [3].

[1] M. Hinczewski et al., J. Chem. Phys. 132, 245103 (2010)
[2] Y. von Hansen et al., Phys. Rev. E 84, 051501 (2011)
[3] F. Sedlmeier et al., J. Stat. Phys. 145, 240-252 (2011)

CPP 16.45 Tue 18:15 Poster A

Fundamental measure density functional for the soft sphere erf-model — •Markus Burgis and Matthias Schmidt — Theoretische Physik II, Physikalisches Institut, Universitaet Bayreuth, D-95440 Bayreuth

As a generic model for soft colloids we consider a fluid of repulsive particles where the Mayer bond is a superposition of two error functions, which allows to interpolate between hard spheres and Gaussian cores. The corresponding pair interaction potential contains the colloidal size and the length scale over which the soft repulsion decays. We deconvolve the Mayer bond for general mixtures of such particles into single particle weight functions. Both the soft sphere weight functions and the Kierlik-Rosinberg scalar hard sphere weight functions follow from a set of coupled partial differential equations, where first derivatives with respect to the geometric model parameters are related to (multiple) application of the Laplace operator in position space. Rescaling the length scales in the weight functions allows to construct an accurate star approximation to the exact triangle diagram in the virial series. Corresponding scaling and exploiting isometric transformations of the weight functions leads to a fundamental measure free energy density functional for the pure fluid. Considering cases where the particle core is effectively impenetrable, we calculate the bulk fluid radial distribution function via the Ornstein-Zernike route. Comparison to results from our Monte Carlo simulations demonstrates over a broad range of densities that the theory accurately reproduces the loss of liquid structure upon increasing softness of the repulsion.

CPP 16.46 Tue 18:15 Poster A

DFT-reconstructed photoelectron spectra for metals in ionic liquids — •Markus Reinmöller, Angela Ulbrich, André Zühlsdorff, Stefan Krischok, Erich Runge, and Wichard J. D. Beenken — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Postfach 10 05 65, D-98684 Ilmenau

Metal atoms in ionic liquids (ILs) have gained interest for catalytic and electrochemical applications as well as an alternative route to generate nanostructures. Furthermore, alkali metal containing ILs may be utilized for storage of electrical energy. The combination of metals and an ionic liquid can be established in several ways: metal atoms may be deposited onto the IL, (electrochemically) dissolved in the IL or chemically bonded to the IL. In the present study copper and alkali metals like potassium are studied, which have been deposited (from vapour) onto the ionic liquid. To keep charge and spin balanced we have calculated clusters of ions and metal atoms by DFT and reconstructed the respective photoelectron spectra for core levels and valence band [1]. The theoretical spectra of the model systems have been compared to experimental photoelectron spectra (XPS, UPS).

[1] M. Reinmöller et al., Phys. Chem. Chem. Phys., 13 (2011) 19526.