

CPP 45: Colloids and Complex Liquids II

Time: Thursday 15:00–18:45

Location: H40

Invited Talk

CPP 45.1 Thu 15:00 H40

Interacting colloidal fluids self-assembled from supramolecular polymers — TINGZI YAN¹, KLAUS SCHRÖTER¹, FLORIAN HERBST², WOLFGANG BINDER², and •THOMAS THURN-ALBRECHT¹ — ¹Institute of Physics, Martin-Luther University Halle-Wittenberg — ²Institute of Chemistry, Martin-Luther University Halle-Wittenberg

It is well established that small or medium sized molecules carrying groups with specific interactions can form supramolecular polymers and networks. In many cases, the specificity of the underlying interactions is most prominent in dilute solution. We present a supramolecular system based on polyisobutylene polymers with thymine and 2,6-diaminotriazine functional end groups forming well-defined micellar aggregates in the melt whose properties can be described as that of an interacting colloidal fluid. The concentration of micelles depends on temperature leading to a solid-fluid ordering transition for monofunctional polymers which shows up in structure as well as in the rheological properties. Bifunctional polymers on the other hand can form hydrogen-bonds between micelles leading to a temperature dependent solidification by gelation without ordering.

CPP 45.2 Thu 15:30 H40

New particle-to-mesh scheme for modeling high-molecular weight dense polymer systems — •GUOJIE ZHANG¹, KOSTAS CH. DAOULAS^{1,2}, and KURT KREMER¹ — ¹Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — ²Innovation Lab GmbH, Speyerer Straße 4, 69115 Heidelberg, Germany

We consider a recently proposed model of high-molecular weight polymeric systems representing the molecules by chains of soft spheres with fluctuating size. Within this description, we develop a grid-based Monte Carlo method for efficient modeling of polymer melts. The soft spheres represent Gaussian density distributions of segments of underlying microscopic sub-chains. The coordinates and the radii of the spheres are defined in continuum space and simple bonded potentials keep the chain connectivity. The non-bonded interactions are defined via a discretized functional of the local density, obtained by mapping the density clouds of the spheres onto a grid, without requiring a neighbor list. The accuracy of the method is verified by comparing the results of the grid-based simulations with data obtained from a standard potential-based description. In contrast to most lattice-based descriptions, the approach allows for simulations in the isothermal-isobaric ensemble. Subsequently, the perspectives of the new scheme for creating equilibrated configurations of long polymer melts with microscopic level of detail are discussed. For this purpose, we introduce a hierarchical strategy increasing gradually the resolution of the model.

CPP 45.3 Thu 15:45 H40

Clustering in β -lactoglobulin and lysozyme protein solutions studied by SAXS — •BO JING¹, FAJUN ZHANG¹, FELIX ROSEN-RUNGE¹, MICHAEL SZTUCKI², and FRANK SCHREIBER¹ — ¹Institute of Applied Physics, University of Tübingen — ²ESRF, Grenoble, France

The understanding of protein cluster formation provides insight into protein function, crystallization and protein aggregation induced diseases. β -lactoglobulin (BLG) is known to form dimers, tetramers, hexamers and octamers at certain pH, temperature, and salt concentrations. Here, we present SAXS measurements which indicate oligomer formation at high protein concentrations, in the absence of salt and other additives. Scattering curves of BLG solutions display a major correlation peak which shifts minimally to higher q -values with increasing protein concentration. This observation is indicative of cluster formation or, in this case, oligomerization. We draw a comparison with the well-studied lysozyme protein system, where we observed a more pronounced shift of the major correlation peak that has been associated with the formation of a dynamical cluster phase. In this system, the peak position also shows a temperature dependence not seen with BLG solutions. The SAXS data of both systems were fitted to elliptical form factors and two-Yukawa interaction potentials. We relate the different clustering models and contrasting temperature responses in these protein systems to differences in their interaction potential and the distinct properties of BLG and lysozyme proteins molecules. In this context, the shortcomings of isotropic interaction models and the

need to consider patchy interactions are also discussed.

CPP 45.4 Thu 16:00 H40

Finding Colloidal Hard Spheres — MARKUS FRANKE¹, ACHIM LEDERER¹, SEBASTIAN GOLDE¹, ECKHARD BARTSCH², and •HANS JOACHIM SCHÖPE^{1,3} — ¹Johannes Gutenberg Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Germany — ²Albert-Ludwigs-Universität Freiburg, Institut für Physikalische Chemie, Albertstr. 21, 79104 Freiburg — ³Max-Planck-Institut für Polymerforschung, Postfach 3148, 55021 Mainz, Germany

In two recent publications it was claimed that there are difficulties in the preparation and characterization of colloids with hard sphere (HS) like interaction [1, 2]. Using PMMA-PHSA particles dispersed in organic solvents serious deviations from the ideal HS behavior have been observed. Furthermore the authors are of the opinion that in general the experimental determination of the particle volume fraction suffers from an inaccuracy of 0.03 to 0.06. Using highly cross linked polystyrene particles dispersed in ethylnaphtalene an optical and gravity matched colloidal model system with HS like interaction can be realized. We performed a comprehensive characterization of our colloidal model system giving us the possibility to determine the particle volume fraction with an accuracy better than 0.01. Analyzing different physical properties (sedimentation velocity, equilibrium phase behavior, crystallization kinetics, equilibrium lattice constant, glass transition dynamics, collective diffusion, short time diffusion) over a large volume fraction range (0.01 up to 0.74) we can show that this particles monitor HS behavior over the entire concentration range. [1] *Soft Matter* 8, 21 (2012), [2] *Soft Matter* 9, 17 (2013)

CPP 45.5 Thu 16:15 H40

How elasticity influences the dynamics of bead-spring-chains in shear flow — •JOHANNES GREBER and WALTER ZIMMERMANN — LS Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth

Simulations of dumbbells in shear flow show that in the semi-diluted regime of a dumbbell suspension individual dumbbells make flips after unpredictable time intervals [1].

With the help of the Fluid Particle Dynamics (FPD) we simulate suspensions of flexible dumbbells corresponding to high Weissenberg numbers Wi and low Reynolds numbers Re [2,3]. We investigate how the flexibility of springs connecting the two beads of a dumbbell (measured by Wi) influences the mixing behaviour in a dumbbell suspension. Further we compare the dynamics of the flow of a dumbbell suspension with the turbulent flow regime in Newtonian fluids at high Reynolds numbers.

References

- [1] J. Bammert et al. (preprint)
- [2] H. Tanaka and T. Araki, *Phys. Rev. Lett.* 85, 1338 (2000)
- [3] P. Peyla, *EPL* 80, 34001 (2007)

CPP 45.6 Thu 16:30 H40

Shear-induced diffusion of spheroidal particles in non-Brownian suspensions at low Reynolds numbers — •FLORIAN JANOSCHEK, FEDERICO TOSCHI, and JENS HARTING — Eindhoven University of Technology, Eindhoven, The Netherlands

Hydrodynamic diffusion can strongly enhance mass and heat transport in microfluidic systems. However, while several authors discussed the shear-induced self-diffusion of spherical particles in experiment, theory, and simulation at low or vanishing Reynolds numbers, less is known about the case of non-spherical particles that are present in suspensions as different as blood, mud, or paint. We present our numerical study of concentrated suspensions of rigid particles at different oblate and prolate aspect ratios. The hydrodynamic self-diffusion is compared with the one obtained for spherical particles and the effect of asphericity at varying volume fractions is discussed.

15 min break

CPP 45.7 Thu 17:00 H40

Gold Nano Rods Close to Charged and Uncharged Surfaces: Slowing Down of Rotational and Translational Diffusion — •MARYAM HAGHIGHI¹, MUHAMMAD NAWAZ TAHIR², WOLFGANG TREMEL², HANS-JÜRGEN BUTT¹, and WERNER STEFFEN¹ —

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Diffusion and rotation of gold nanorods close to a solid interface were studied with two recently introduced techniques: Resonance Enhanced Dynamic Light Scattering (1) and Waveguide Enhanced Dynamic Light Scattering (2). We observed strong, plasmon-enhanced light scattering. Gold nano rods were stabilized by cetyltrimethylammonium bromide (CTAB). They showed an unexpected strong slowing down of the translational diffusion coefficient, whereas for rotational diffusion this slowing down is distinct but less pronounced. To find the possible influence of charges on the solid interface on this slowing we varied the added salt concentration. Another approach was to cover the metal interface with an electrically neutral layer of poly-methylmethacrylate. A third approach was to completely exchange CTAB for its covalently bound, thiolated analogue 16-mercaptohexadecyl trimethylammonium bromide (MTAB), this reduces the slowing down considerably. (1) Plum MA, Menges B, Fytas G, Butt HJ, Steffen W, Rev. Sci Instr. 2011, 82, 015102 (2) Plum MA, Vianna SDB, Unger A, Roskamp RF, Butt HJ, Menges B, Steffen W, Soft Matter 2011, 7, 1501

CPP 45.8 Thu 17:15 H40

Phase behavior of colloidal monolayers on one-dimensional periodic light potentials — ●LAMISS ZAIDOUNY, THOMAS BOHLEIN, 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 inter-particle forces and their interaction with the substrate, interesting structures will form which are also observed in atomic systems. Here, we study the phase transitions of charged colloidal particles on arrays composed of periodic one-dimensional laser lines which are created by a scanned laser beam. The colloidal particles used are suspended in an organic solvent with low polarity that causes the formation of spontaneous hexagonal crystals of large lattice constants as compared to those formed in aqueous solutions. This fact provided a new regime where phase transitions are accessed for different periods of the light patterned substrates.

CPP 45.9 Thu 17:30 H40

Percolation thresholds and critical exponents of colloidal suspensions in bulk and confinement — ●HELGE NEITSCH and SABINE H. L. KLAPP — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

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

- [1] H. Neitsch and S. H. L. Klapp, submitted, arXiv:1211.1027 (2012)
 [2] P. J. Lu, E. Zaccarelli, F. Ciulla, A. B. Schofield, F. Sciortino, and D. A. Weitz, Nature **453**, 499 (2008)
 [3] R. L. C. Vink, K. Binder, and J. Horbach, Phys. Rev. E **73**, 056118 (2006)

CPP 45.10 Thu 17:45 H40

Confinement induced repulsion in oscillatory structural forces — ●SEBASTIAN SCHÖN and REGINE VON KLITZING — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Straße des 17. Juni 124, D-10623 Berlin

Suspensions of nanoparticles show a layered ordering in the vicinity of surfaces. Overlap of these regions, as under confinement conditions,

leads to oscillatory changes in the ordering behavior of the particles, dependent on the exact wall to wall distance. These changes originate from the entropic excluded volume effect and indicate a break in the translational symmetry of the bulk system.

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 from the deflection signal of the cantilever and are normalized with the radius of the colloidal probe to get the corresponding force curves. These provide a direct means to the structural response of the nanoparticles during a gradual change of the confinement.

Investigation of suspensions with varying ionic strength and pH, invoked via addition of sodiumchloride, sodiumhydroxide or hydrochloric acid, show an additional repulsion underlying the normal structural force signal as described by Israelachvili. The key parameters of the oscillatory force signal, namely amplitude, wavelength and decay-length as well as the extra repulsion are compared for suspensions with different additives.

CPP 45.11 Thu 18:00 H40

Phase transitions and phase equilibria in spherical confinement — ●ANTONIA STATT, ALEXANDER WINKLER, PETER VIRNAU, and KURT BINDER — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

The interplay of finite size and surface effects for fluids confined in a sphere is studied via Monte Carlo simulations of the Asakura-Oosawa model for colloid-polymer mixtures¹ using free energy calculations. For this model the phase separation in a colloid-rich phase and a polymer-rich phase is well known in the bulk^{2,3} and we show that spherical confinement enhances the miscibility of the mixture. Depending on the wall potentials of the confining surface, the wetting properties can be controlled, and this interplay between adsorption of one species to the confining surface and bulk unmixing leads to very special shapes of the loops observed for the chemical potential of the colloids.

- [1] S. Asakura and F. Oosawa, J. Polym. Sci. **33**, 183
 [2] R.L.C. Vink and J. Horbach, J. Chem. Phys. **121**, 3253
 [3] R.L.C. Vink, J. Horbach, and K. Binder, Phys. Rev. E **71**,011401

CPP 45.12 Thu 18:15 H40

Fluids in extreme confinement — ●THOMAS FRANOSCH¹, SIMON LANG¹, and ROLF SCHILLING² — ¹Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058, Erlangen, Germany — ²Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

For extremely confined fluids with two-dimensional density n in slit geometry of accessible width L , we prove that in the limit $L \rightarrow 0$ the lateral and transversal degrees of freedom decouple, and the latter become ideal-gas-like [1]. For small wall separation the transverse degrees of freedom can be integrated out and renormalize the interaction potential. We identify nL^2 as hidden smallness parameter of the confinement problem and evaluate the effective two-body potential analytically, which allows calculating the leading correction to the free energy exactly. Explicitly, we map a fluid of hard spheres in extreme confinement onto a 2d-fluid of disks with an effective hard-core diameter and a soft boundary layer [1]. Two-dimensional phase transitions are robust and the transition point experiences a shift $O(nL^2)$.

- [1] Thomas Franosch, Simon Lang, and Rolf Schilling, Phys. Rev. Letter (2012) in press

CPP 45.13 Thu 18:30 H40

Coarse-graining strategies for coronene molecules — ●THOMAS HEINEMANN and SABINE H. L. KLAPP — Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Coarse-graining describes the idea of systematically integrating out irrelevant degrees of freedom in order to create an effective Hamiltonian, which allows to investigate larger length- and time scales. In this contribution we focus on the coarse-graining of coronene molecules from atomistic detail to mesoscopic molecular detail. So far only a complicated, temperature-independent coarse-grained model for coronene, used for static calculations, exists [1].

A hierarchy of model potentials generating different many-particle aspects of coronene, e.g. crystal stability, aggregation, etc., will be introduced. These models are studied via mesoscopic Molecular Dynamics simulations. As a basic platform for molecular pair interactions, the Gay-Berne potential with electric multipoles (GBEMP), which has been established [2], is used. This ansatz is combined with param-

eters characterizing the electronic contributions as well as shape contributions from atomistic, biased Umbrella Sampling simulations. The fitting procedure of the models will be discussed.

- [1] O. I. Obolensky et al., *Int. J. Quantum Chem.* 107 (2007) 1335.
- [2] P. Xu et al., *J. Mol. Model.* (2012), doi:10.1007/s00894-012-1562-5.