CPP 36: Colloids and Complex Fluids II (joint session BP/CPP/DY, organized by CPP)

Time: Wednesday 10:15–13:00 Location: ZEU 260

Invited Talk CPP 36.1 Wed 10:15 ZEU 260

Computer simulations of colloidal systems under flow — •Arash Nikoubashman — Institut für Physik, Johannes Gutenberg-Universität Mainz, Mainz, Germany

Colloidal systems under flow are ubiquitous in nature and technology, whether it is the transport of proteins and enzymes in biological systems or the flow of surfactants in enhanced oil recovery. Such microrheological systems are also highly intriguing from a purely scientific point of view due to the intricate interplay between the solute and solvent particles. To better understand the physical properties of these complex systems and to assist the design of microfluidic devices, we performed extensive simulations of both rigid and soft colloidal particles under flow. This computational approach allows for systematic control over the system parameters while also providing microscopic insight. In this presentation, selected systems will be discussed to give an overview of the possibilities and challenges in this field. For example, microfluidic channels can be used to distinguish polymers based on their topology, such as linear, dendritic or ring-shaped macromolecules. Furthermore, non-linear flow effects such as inertia or viscoelasticity can be exploited to control the lateral motion of dispersed particles. Flow can also be used to enhance the growth as well as the breakup of colloidal aggregates, depending on the applied flow strength.

CPP 36.2 Wed 10:45 ZEU 260

A temporarily arrested state in protein solutions — •Stefano Da Vela[1], Fajun Zhang[1], Christian Exner[1], Johannes Möller[2], Zhendong Fu[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France — [3]JCNS, Garching, Germany

The interplay of liquid-liquid phase separation (LLPS) with the glass transition is a possible route to the formation of arrested states in colloidal and protein systems. LLPS requires attractive interactions, the microscopic details of which set the temperature dependence of the LLPS phase boundary. We report the kinetics of phase separation and arrest for two protein systems: γ-globulin in the presence of PEG 1000, featuring upper critical solution temperature behavior, and bovine serum albumin in the presence of Y(III), featuring lower critical solution temperature behavior. For both systems, the time evolution of the characteristic length is followed during phase separation by Ultra Small Angle X-ray Scattering (USAXS) and Very Small Angle Neutron Scattering(VSANS). This time evolution corresponds to classical LLPS proceeding by spinodal decomposition for shallow quenches in the two-phase region, and to arrested LLPS for deep enough quenches [1]. For intermediate quenches, we report evidence of an unusual three-stage coarsening process. In this case, a temporary arrest of the kinetics is found, which is overcome at later times. We interpret the finding in the light of simulations and experimental results on colloidal systems.

[1] Da Vela et al. Soft Matter, 2016, 12, 9334 - 9341

CPP 36.3 Wed 11:00 ZEU 260

Demixing and clustering in a binary system of long-ranged capillary interactions — •Malte Lütje, Johannes Bleibel, and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen, Deutschland

We consider a binary system of micron-sized spherical colloidal particles trapped at a fluid interface, which induces long-ranged capillary interactions. If one species has positive and one has negative buoyancy, colloids of the same species attract while different species repel. This leads to the demixing of initially uniform densities, and ultimately to the formation of close-packed clusters for each species. Demixing competes with the clustering of each species.

We present static phase diagrams for the system. Brownian Dynamics simulation results illustrate the evolution from a homogeneous state to the demixed and clustered states. The system has unusual phase separation dynamics: The timescales of demixing and clustering can be different, yielding an intermediate stage with halo-like structures.

CPP 36.4 Wed 11:15 ZEU 260

Poisson-Boltzmann study of the effective electrostatic interaction between colloids at an electrolyte interface — •Arghya Majee[1,2], Markus Bier[1,2], and S. Dietrich[1,2] — [1]Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569, Stuttgart — [2]IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart

The effective electrostatic interaction between a pair of colloids, located close to each other at an electrolyte interface, will be discussed by employing the full, nonlinear Poisson-Boltzmann (PB) theory within classical density functional theory. Using a simplified yet appropriate model, all contributions to the effective interaction are obtained exactly, albeit numerically. The comparison between our results [1] and those obtained within linearized PB theory [2] reveals that the latter overestimates these contributions significantly at short inter-particle separations. Whereas the surface contributions to the linear and the nonlinear PB results differ only quantitatively, the line contributions show qualitative differences at short separations. Moreover, a dependence of the line contribution on the solvation properties of the two adjacent fluids is found, which is absent within the linear theory. Our results are expected to enrich the understanding of effective interfacial interactions between colloids.

References:

[1] A. Majee, M. Bier, and S. Dietrich, J. Chem. Phys. **145**, 064707 (2016). [2] A. Majee, M. Bier, and S. Dietrich, J. Chem. Phys. **140**, 164906 (2014).

15 min break

CPP 36.5 Wed 11:45 ZEU 260

Entropic Interactions between Dendrimers and Impenetrable Surfaces — •Ron Dockhorn[1,2], Stephan Meschede[3], Martin Wengenmayr[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — [3]Institute for Physics, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany

Monte Carlo simulations are performed to investigate depletion effects on dendrimers using the bond fluctuation model. Two different situations are investigated: The interaction between a single dendrimer against a hard wall and the interaction between two dendrimers. The simulations of the dendrimers are performed with implicit solvent as well as in a linear polymer matrix. The free energy landscape along the particular reaction coordinate is determined by Umbrella Sampling (WHAM algorithm) and compared to a mean-field approach. Both systems immersed in a polymer matrix show entropic attraction (depletion forces) depending on the length of the surrounding linear chains. Additionally, a spontaneous conformational change and rapid mixing caused by the strong interaction in the two dendrimers' system can be noticed. These findings are aimed to understand the agglomeration and the coagulation processes of hyperbranched structures in drug-delivery systems in medical applications.

CPP 36.6 Wed 12:00 ZEU 260

Liquid-state theory of the interactions between colloids mediated by attractive reversibly adsorbed polymers. — •A.I. Chervanyov — Institute for Nano- and Microfluidics, TU Darmstadt

By making use of the liquid state theory, we analytically study the effect of attractive polymer-colloid (P-C) and polymer-polymer (P-P) interactions on the effective forces acting between colloids immersed in a polymer system. The performed theoretical analysis has no restrictions with respect to the polymer density and relative sizes of the colloids and polymers. The polymer mediated (PM) potential acting between fillers is shown [1,2] to significantly depend on the strength and range of the P-P and P-C interactions. In the nano-particle limit, where the colloid radius is much smaller than the polymer gyration radius, the presence of attractive P-P interactions causes significant, but only quantitative changes to the PM potential. In the opposite limit of relatively large colloids, the P-P interactions revert the sign of the total effective force acting between colloids so that this force becomes attractive at sufficiently large polymer densities. The effect of the C-P interactions on the PM potential is found to be most pronounced in the case of large polymer densities and small colloid-to-polymer size ratios. The dependence of the second virial coefficient of the effective PM potential on the polymer density is discussed in detail, revealing several novel features of the PM forces caused by the presence of attractive P-P and P-C interactions.

[1] A.I. Chervanyov, Soft Matter 11,1038-1053 (2015).
[2] A.I. Chervanyov, J. Chem. Phys. 141, 244902(2014).

CPP 36.7 Wed 12:15 ZEU 260

Determing helicity modulus in systems with orientational order from microscopic properties through Zwanzig-Mori formalism — •Johannes Häring and Matthias Fuchs — FB Physik, Universität Konstanz, 78457 Konstanz, Germany

Up to now, we have studied crystals with point disorder and applied the theory to crystals of soft core particles, so-called cluster crystals [1]. Now, systems with orientational order like nematic liquid crystals are considered. With the Zwanzig-Mori formalism it is possible to calculate the helicity modulus for all temperatures in the ordered phase, even near the critical point.

The Zwanzig-Mori formalism is a way to treat many-body systems systematically. Projection Operators are used to focus on the dominant variables of the system and their correlation functions. Simulations of the three dimensional XY model are done to test the accuracy of the approach. The XY model consists of particles with one orientational degree of freedom which are fixed on a lattice.

It is known from the Mermin-Wagner theorem that two dimensional systems show no conventional long range order, i.e have vanishing order parameters. That leads to problems in calculating the helicity modulus. We discuss how it is still possible to obtain a solution.

[1] J. M. Häring, C. Walz, G. Szamel, and M. Fuchs, Phys. Rev. B 92, 184103 (2015)

CPP 36.8 Wed 12:30 ZEU 260

Clusters in dipolar fluids — •Michela Ronti[1], Alexey O. Ivanov[2], Lorenzo Rovigatti[3], Jose M. Tavares[4], Francesco Sciortino[5], and Sofia S. Kantorovich[1,2] — [1]Computational Physics, University of Vienna, Sensengasse 8, 1090 Vienna, Austria — [2]Ural Federal University, 3 Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford, OX1 4 NP, United Kingdom — [4]Instituto Superior de Engenharia de Lisboa-ISEL, Rua Conselheiro Emidio Navarro 1, 1950-062 Lisboa, Portugal — [5]University of Rome La Sapienza, Piazzale Aldo Moro 2, I-00185, Roma, Italy

We describe the self-assembly in magnetic nanocolloids by using a dipolar hard sphere (DHS) model. The phase diagram of this system at low temperature remains debatable regardless the expected simplicity of the model. At low temperature DHS particles self-assemble into complex structures, with primary structures composed by rings and chains. The latter form the building blocks for further aggregation. To elucidate the formation of branched structures analytically, we need to calculate accurately partition functions of various clusters. For that we introduce grand-canonical single cluster Monte Carlo simulations.

CPP 36.9 Wed 12:45 ZEU 260

Ferromagnetic phases in colloidal suspensions — •Grigorii Zarubin[1,2] and Markus Bier[1,2] — [1]Max Planck Institute Int. Sys. — [2]University of Stuttgart, Germany

A ferromagnetic phase of anisotropic particles suspended in a nematic liquid crystal (NLC) was predicted as early as 1970 [1]. A recent experimental realization [2] confirmed that a dilute suspension of magnetic platelets in NLC forms ferromagnetic phase which is susceptible to weak magnetic fields. In this work we describe such a suspension of plate-like particles using density functional theory. The influence of the NLC is taken into account implicitly through the introduction of the effective elastic interaction between platelets. Following approach of Lev and Tomchuk [3], the effective potential was derived under the assumption of weak anchoring of the NLC at the surface of the platelets. An ordered phase was identified with help of the orientational distribution function, and the dependence of the ferromagnetic phase on the strength of the magnetic and the elastic coupling was studied.

References: [1] F. Brochard and P.G. de Gennes, J. Physique 31, 691 (1970). [2] A. Mertelj, D. Lisjak, M. Drofenik and M. Copic, Nature 504, 237 (2013). [3] B.I. Lev and P.M. Tomchuk, Phys. Rev. E 59, 1 (1998).