CPP 24: Colloids and Complex Fluids I (joint session BP/CPP/DY, organized by CPP)

Time: Tuesday 11:30–13:00   Location: ZEU 255

CPP 24.1 Tue 11:30 ZEU 255
Small activity differences drive phase separation in polymers — •JAN SMREK and KURT KREMER — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Recent theoretical studies found that mixtures of active and passive colloidal particles phase separate but only at very high activity ratio. The high value poses serious obstacles for experimental exploration of this phenomenon. Here we show using simulations that when the active and passive particles are *polymers*, the critical activity ratio decreases with the polymer length. This not only facilitates the experiments but also has implications on the DNA organization in living cell nuclei. Entropy production can be used as an accurate indicator of this non-equilibrium phase transition.

CPP 24.2 Tue 11:45 ZEU 255
Corresponding States Law For Protein Solutions — •FLORIAN PLATTEN and STEFAN U. EGELHAAF — Heinrich Heine University, Condensed Matter Physics Laboratory, Duesseldorf, Germany

The extended law of corresponding states, as proposed by Noro and Frenkel, involves a mapping of the phase behavior of systems with short-ranged attractions. We test its applicability to protein solutions with their complex interactions. We successfully map the experimentally determined metastable gas-liquid binodals to the binodals of short-ranged square-well fluids. This is achieved by representing the binodals as a function of the temperature scaled with the critical temperature (or as a function of the reduced second virial coefficient) and the concentration scaled by the cube of an effective particle diameter, where the scalings take into account the attractive and repulsive contributions to the interaction potential, respectively. The scaled binodals of the protein solutions coincide with simulation data of the adhesive hard-sphere fluid. Furthermore, once the repulsive contributions are taken into account by the effective particle diameter, the temperature dependence of the reduced second virial coefficients follows a master curve that corresponds to a linear temperature dependence of the depth of the square-well potential. We moreover demonstrate that, based on this approach and cloud-point measurements only, second virial coefficients can be estimated, which we show to agree with values determined by light scattering or by Derjaguin-Landau-Verwey-Overbeek (DLVO)-based calculations.

Platten et al., J. Chem. Phys. 142, 174905 (2015).

CPP 24.3 Tue 12:00 ZEU 255
Critical Casimir interactions between Janus particles — •MARCEL LABBÉ-LAURENT and SIEGFRIED DIETRICH — Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Critical fluctuations in binary liquid mixtures give rise to forces acting on immersed colloidal particles. Experiments have demonstrated a remarkable agreement with theoretical predictions for spherical colloids close to a (chemically patterned) substrate [1,2]. At the same time, there has been strong experimental and theoretical interest in studying the self-assembly and the phase behavior of patchy and Janus particles. Although a variety of effective interactions have been proposed to drive the self-assembly, the critical Casimir effect stands out as being particularly suitable because it provides both attractive and repulsive interactions depending on the chemical surface properties, as well as a sensitive control of their strength via minute temperature changes. We present theoretical calculations for the interaction between a single Janus particle and a chemically structured substrate and the effective pair potential between two Janus cylinders as well as between two Janus spheres [3].

[1] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich, and C. Bechinger, *Nature* **451**, 172 (2008).
[2] M. Tröndle, O. Zvyagolskaya, A. Gambassi, D. Vogt, L. Harnau, C. Bechinger, and S. Dietrich, *Mol. Phys.* **109**, 1169 (2011).
[3] M. Labbé-Laurent, and S. Dietrich, *Soft Matter* **12**, 6621 (2016).

CPP 24.4 Tue 12:15 ZEU 255
From criticality to gelation in sticky spheres — DAVID RICHARD[1,2], THOMAS SPECK[1], and •CRISTOPHER PATRICK ROYALL[2]

— [1]Institut fur Physik, Johannes Gutenberg-Universitat, Mainz, Germany — [2]HH Wills Physics Laboratory, Tyndall Avenue, Brisol, United Kingdom

Understanding the mechanism of dynamical arrest in liquids is a long standing challenge. Even for simple fluids, such as sticky spheres, an arrested gel can occur when the system is quenched sufficiently fast such that it cannot relax to equilibrium. For many systems the gelation arises at the gas-liquid phase boundary, forming a rigid but dilute network of bonded particles. In this study, we look at the critical behavior of sticky spheres combining confocal microscopy of colloid-polymer mixtures and Monte Carlo simulations of the square-well model. The mapping between those two is achieved via tracking colloids at the single-particle level and fitting pair distribution functions to the simulation data. We then compare the local structure via the topological cluster classification (TCC) method to identify locally favored structures (LFSs) along the critical path. We observe a very good agreement between experiments and simulations, where the growth of highly ordered structures are triggered even far away from the phase boundary. We discuss the link of those LFSs to the global percolating bond network.

CPP 24.5 Tue 12:30 ZEU 255
Determination of crystal nucleation barriers for colloidal crystals from computer simulations — •PETER KOSS[1,2], ANTONIA STATT[3], PETER VIRNAU[1], and KURT BINDER[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Princeton University, Princeton, NJ 08544, USA

A fluid in equilibrium, confined in a finite volume, with a density exceeding the onset of freezing, may exhibit phase coexistence with a crystal nucleus surrounded by liquid or a gas. Classical nucleation theory predicts that the barrier of homogeneous nucleation is given by two contributions, the free energy gained by the creation of a crystal droplet and the free energy loss due to surface tension of the newly created interface. We obtain the excess free energy due to the surface of the crystalline nucleus by using a computational method suitable for the estimation of the chemical potential of dense fluids. Our analysis method is appropriate for crystal nuclei of all shapes, without suffering from ambiguities occurring when one needs a microscopic identification of the crystalline droplet. We present a novel analysis method to determine the coexistence pressure between fluid and crystal, and report that the nucleation barrier for a soft version of the effective Asakura-Oosawa model is compatible with a spherical shape, and consistent with classical nucleation theory [1].

[1] A. Statt, P. Virnau, and K. Binder, Phys. Rev. Lett. 114, 026101 (2015).

CPP 24.6 Tue 12:45 ZEU 255
Phonons and Elasticity in Disordered binary Crystals — •TADEUS RAS and MATTHIAS FUCHS — FB Physik, Univ. Konstanz

The "method of long waves" is a well-established tool for the study of elastic constants [1]. However, until recently, it had been lacking in crystals with point defects due to an unclear definition of the displacement field.

We present a generalization of the projection-operator approach employed in [2]. It yields expressions for the elastic constants valid in binary crystals with arbitrary amounts of point defects and up to the melting temperature. Further, both acoustic and optical phonon eigenfrequencies can be computed in linear response.

While density functionals from classical DFT serve as an input parameter to the approach it can also be employed experimentally to process measurement data. For demonstration, dispersion relations will be shown as obtained from molecular dynamics data of a hard sphere model crystal [3].

[1] D. C. Wallace, Thermodynamics of Crystals (Wiley, NY 1972).
[2] C. Walz and M. Fuchs, Phys. Rev. B **81**, 134110 (2010).
[3] L. Filion et. al., Phys. Rev. Lett. **107**, 168302 (2011).