

## CPP 40: Colloids and Complex Liquids III

Simulation/Theory

Time: Thursday 11:15–12:45

Location: ZEU 260

CPP 40.1 Thu 11:15 ZEU 260

**Dynamical signatures of length-scale dependent hydrophobic hydration** — ●RICHARD GREGOR WEISS<sup>1</sup> and JOACHIM DZUBIELLA<sup>1,2</sup> — <sup>1</sup>Humboldt Universität zu Berlin — <sup>2</sup>Helmholtz-Zentrum Berlin

We present an investigation of the curvature dependence of water dynamics at hydrophobic solutes by using Molecular Dynamics simulations of SPC/E water at differently sized spherical model surfaces.

As an important novel insight into the subject we present the dependence of water molecule mobility on surface curvature. The findings show that the diffusional behavior and the sojourn times of water molecules at hydrophobic surfaces strongly depend on surface curvature. In addition the curvature dependence exhibits a non-monotonic progression as it is already known for water hydration structure [1].

Our study demonstrates the existence of an intimate connection between static and dynamic curvature effects of hydrophobic hydration. Large implications arise for the interpretation of dynamical measurements of hydration at heterogeneous biomolecular surfaces with varying surface geometry.

[1] D. Chandler, vol. 437, pp 640-647, Nature

CPP 40.2 Thu 11:30 ZEU 260

**Alignment of cylindrical colloids induced by critical Casimir torques** — ●MARCEL LABBÉ-LAURENT<sup>1,2</sup>, MATTHIAS TRÖNDLE<sup>1,2</sup>, LUDGER HARNAU<sup>1,2</sup>, and SIEGFRIED DIETRICH<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart — <sup>2</sup>IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Critical fluctuations in simple fluids or binary liquid mixtures give rise to forces acting on immersed colloidal particles. These Casimir-like forces are attractive or repulsive depending on the chemical surface properties [1]. Recent experiments have demonstrated a fluctuation-induced lateral trapping of spherical colloidal particles immersed in a binary liquid mixture near its critical demixing point and exposed to chemically patterned substrates [2].

Inspired by these experiments, we study the critical Casimir effect for elongated colloids of cylindrical shape. When the colloidal particles are close to a chemically structured substrate, a critical Casimir torque acting on the colloids emerges. Our analysis indicates that critical Casimir interactions are capable to achieve well-defined, reversible alignments both of chemically homogeneous and of Janus cylinders [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, M. Tröndle, L. Harnau, S. Dietrich, preprint; arXiv:1311.3814 (2013)

CPP 40.3 Thu 11:45 ZEU 260

**Fundamental measure approaches to liquid crystals** — ●RENÉ WITTMANN, MATTHIEU MARECHAL, and KLAUS MECKE — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Fluids of hard spherocylinders exhibit a rich phase behavior including isotropic, nematic and smectic-A phases. A density functional for anisotropic hard bodies can be constructed in terms of tensorial weighted densities (FMT) which depend on geometry and position of only one single oriented particle [1]. Within a new geometric method to derive the exact low-density functional we introduce a mixed measure of two bodies which can be expanded to the original tensor series. We compare this fundamental mixed measure theory (FMMT) to approximated results and Monte-Carlo simulations.

Closed formulas for the Frank elastic coefficients and the restriction to parallel spherocylinders verify the consistency of FMMT analytically. The isotropic - nematic interfacial tension remarkably improves on earlier, only qualitatively correct predictions [2]. For the first time we obtain a phase diagram of hard spherocylinders which can be quantitatively compared to simulations. We find a first order nematic to smectic-A transition up to an aspect ratio of at least 40. The increased computational effort and the relevance of other components of the functional is discussed.

[1] H. Hansen-Goos and K. Mecke, *Phys. Rev. Lett.* **102**, 018302 (2009).

[2] R. Wittmann and K. Mecke, *J. Chem. Phys.*, submitted (2013).

CPP 40.4 Thu 12:00 ZEU 260

**New Monte Carlo method to simulate interfacial free energies** — ●FABIAN SCHMITZ, PETER VIRNAU, and KURT BINDER — Institut für Physik, Johannes Gutenberg-Universität Mainz, Deutschland

We present a new Monte Carlo simulation method to calculate the interfacial tension  $\gamma$  between two phases, e.g. liquid-gas-coexistence or crystal-liquid coexistence. The knowledge of the precise value of the interfacial tension is of vital importance for the understanding of nucleation phenomena and the prediction of nucleation rates.

The method is based on a thermodynamic integration. In the initial state, the two homogeneous phases are within two completely separate boxes with periodic boundary conditions in all directions. In the final state, the two phases coexist in a joint box and thereby form two interfaces. The free energy difference  $\Delta F$  between the initial and the final state is then given by the surface free energy of the two interfaces. The method is applicable to Ising (lattice gas) models as well as colloidal systems with Lennard-Jones or hard sphere potentials. Since a finite interface has additional entropic terms depending on the box dimensions, a systematic analysis of the finite size effects is carried out.

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**Cluster Formation in Systems of Magnetic Cubes at Low Temperatures.** — ●JOE G. DONALDSON<sup>1</sup> and SOFIA KANTOROVICH<sup>1,2</sup> — <sup>1</sup>Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria — <sup>2</sup>Ural Federal University, Lenin av. 51, Ekaterinburg, 620083, Russia.

Colloidal synthesis has progressed to the point where a large array of particle geometries is now readily accessible. For example, recently realised systems of cubic particles now form an active area of research [Meijer et. al, *Soft Matter*, 2013]. The non-spherical shape of these particles provides a perfect scenario in which to study the consequences of external anisotropy on cluster formation. In addition, an internal anisotropy can be present for particles formed of magnetic compounds. In this work we describe and account for the structures formed in a magnetic cubic colloidal system at low temperatures. Our system is comprised of monodisperse cubes with centrally positioned point magnetic dipoles. Two separate scenarios are considered: one where the dipole orientation is along the [100] crystallographic direction, and the other, along [111]. We present analytical energy calculations in quasi two dimensions of the possible structures formed at 0K. The approach taken here is an extension of that employed for spheres by [Propkopiaeva et. al, *Phys. Rev. E*, 2009]. These predictions are compared to replica exchange molecular dynamics computer simulations at low temperatures. The findings of this work are later hoped to aid in the determination of thermodynamic properties of these colloids at room temperature.

CPP 40.6 Thu 12:30 ZEU 260

**Dynamic States in Driven Liquid Crystals of Hard-Spherocylinders** — ●ELLEN FISCHERMEIER, MATTHIEU MARECHAL, and KLAUS MECKE — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

We investigate a system of hard spherocylinders, arguably the simplest model system for rodlike colloidal liquid crystals, under the influence of an external periodic potential with Langevin dynamics simulation. The chosen potential acts solely on the orientation of each individual particle and represents a preferred direction of alignment which rotates in the x-y-plane. Depending on the rotation frequency of the external potential and the packing fraction of the particles we discover a variety of nonequilibrium states which can be compared to results of density functional theory [1].

We also report on the possibility of coupling this simulation to a Lattice Boltzmann framework to include long range hydrodynamic interactions.

[1] A. Härtel et al., *Phys. Rev. E* **81**, 051703 (2010)