DY 47: Complex Fluids and Soft Matter I (joint session DY/CPP)

Time: Thursday 15:00–16:30 Location: ZEU 160

DY 47.1 Thu 15:00 ZEU 160

All-Atom Molecular Dynamics Simulation of Ionic Liquid films on Silica Surface — •Tamisra Pal and Michael Vogel — Institut für Festkörperphysik,Technische Universität Darmstadt,Hochschulstraße 6 64289 Darmstadt , Germany

Room temperature ionic liquid (RTIL) films in confined geometries have been recognized for their significant interfacial properties in electrochemical and electronic devices. Depending on the hydrophobicity of the anions, we chose IL 1-butyl-3-methylimidazolium cation with hexafluorophosphate ([Bmim][PF6]) and tetrafluoroborate ([Bmim][BF4]) counterparts. Here, the dynamical and structural properties of these ILs confined between amorphous silica slabs have been investigated by all-atom molecular dynamics simulation studies at 300 K. Relative number densities of the ions are calculated near the surface, as well as in the middle of the slit. The more hydrophilic [BF4]- ions tend to stay closer to the slab wall than symmetric [PF6]-, whereas the [Bmim]+ ions always resides in the next layer forming a bi-layered arrangement from the wall. A preferred orientation has been observed for the cations with their methyl groups pointing towards the slab surface and butyl tail projected inwards. The middle of the slit displays more of a bulk behavior in terms of density and ion diffusivities. Spatially-resolved analyses of the mean square displacement (MSD) and incoherent intermediate scattering function (ISF) reveal very sluggish and heterogeneous dynamics of these ILs in the vicinity of the silica surface, which need to be considered when designing applications.

DY 47.2 Thu 15:15 ZEU 160

Kirkwood-Buff integrals in the thermodynamic limit from small-sized molecular dynamics simulations — •Robinson Cortes Huerto, Kurt Kremer, and Raffaello Potestio — Max Planck Institute for Polymer Research, Ackermannweg 10, 55118, Mainz

We present an accurate and efficient method to obtain Kirkwood-Buff (KB) integrals in the thermodynamic limit from small-sized molecular dynamics simulations. By introducing finite size effects into integral equations of statistical mechanics, we derive an analytical expression connecting the KB integrals of the bulk system with the fluctuations of the number of molecules in the corresponding closed system. We validate the method by calculating the activity coefficients of aqueous urea mixtures and the KB integrals of Lennard-Jones fluids. Moreover, our results demonstrate how to identify simulation conditions under which computer simulations reach the thermodynamic limit.

DY 47.3 Thu 15:30 ZEU 160

Reconstruction of phason modes in colloidal quasicrystals — •Johannes Hielscher, Miriam Martinsons, Michael Schmiedeberg, and Sebastian C. Kapfer — FAU Erlangen-Nürnberg, Institut für Theoretische Physik

In colloidal quasicrystals, the idealised positions of the particles can be expressed in higher-dimensional space, accounting for the degrees of freedom of displacements within (phonons), and perpendicular (phasons) to the physical space. Phasonic displacements manifest in "flips", i. e. characteristic particle jumps. Our model systems are two-dimensional intrinsic quasicrystals of decagonal symmetry, which are stabilised by a next-neighbour double-minimum pair potential. Brownian Dynamics and Monte Carlo simulations are conducted to let flip patterns develop at finite temperatures.

We present an method to analyse the flip pattern in a monocrystalline, dislocation-free quasicrystal by decomposition into long-wavelength harmonic phason modes [1]. Thermal flips are only partially accounted for by this approach. We discuss the break-down of the supposed phason-phonon coupling on the atomic scale, in the context of fundamental limitations of extended, collective phasonic distortions in soft quasicrystals with short-range interactions.

[1] J. Hielscher, M. Martinsons, M. Schmiedeberg & S. C. Kapfer: Detection of phonon and phason modes in intrinsic colloidal quasicrystals by reconstructing their structure in hyperspace. *Submitted to J. Phys.: Cond. Matt.*

DY 47.4 Thu 15:45 ZEU 160

Two-step melting in Two Dimensions with Long-ranged forces — •Sebastian Kapfer — Theoretische Physik 1, FAU Erlangen, Germany

Recent progress in global-balance Monte Carlo algorithms has allowed to confirm the essentials of the Halperin-Nelson-Young theory (KTHNY) for the 2D Melting problem with short-range interactions [1]. A key challenge in these simulations are large correlation lengths which could be overcome by a new class of Monte Carlo algorithms [2].

In this talk, I will show that the new Monte Carlo paradigm can be extended to include long-range forces (including periodic images) rigorously, without any truncation effects. The resulting algorithm improves on the scaling of Ewald summation [3].

The new algorithm allows to check the scaling predictions of KTHNY theory in the long-range limit, and complete the phase diagram of inverted power-law potentials, relevant for charged colloids, plasma crystals, and other systems.

[1] S. C. Kapfer & W. Krauth, Phys. Rev. Lett. 114, 035702 (2015). [2] M. Michel et al., J. Chem. Phys. 140, 054116 (2014). [3] S. C. Kapfer & W. Krauth, Phys. Rev. E 94 (R), 031302 (2016).

DY 47.5 Thu 16:00 ZEU 160

Quantised Phase Transition of Confined Discotics forming Concentric Rings: Monte-Carlo and Experimental Studies — •Arne W. Zantop[1], Kathrin Sentker[2], Patrick Huber[2], and Marco G. Mazza[1] — [1]Max-Planck-Institut für Dynamik Komplexer Fluide, Am Faßberg 17, 37077 Göttingen — [2]Institut für Materialphysik und -technologie, Technische Universität Hamburg-Harburg, Eißendorferstr. 42, 21073 Hamburg

Interfaces and geometrical confinement crucially alter the phase transitions of various substances, as those of liquid crystals. We present combined results of a parallel tempering Monte-Carlo study of the discotic Gay-Berne-II fluid model in cylindrical nano-confinement, and an experimental study of the triphenylene derivate HAT6 confined in porous silica pores rendered both hydrophilic and hydrophobic. Here we report a quantised, layer by layer transition of the confined discotic liquid crystals. While the bulk phase shows a discontinuous transition from isotropic to hexagonal columnar phase upon cooling, the confined system forms concentric rings. Starting form the interface these ring develop inwards one after another with a discontinuous increase in local order parameter followed by plateaus with a continuous increase in local order.

DY 47.6 Thu 16:15 ZEU 160

Tracers in complex environments — •Tatjana Sentjabrskaja[1,2], Marco Laurati[3], Viktoria Wollrab[2], Gijsje Koenderink[2], and Stefan Egelhaaf[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]FOM Institute AMOLF, Amsterdam, The Netherlands — [3]Division de Ciencias e Ingenieria, Universidad de Guanajuato, Leon, Mexico

Biological cells are critically dependent on intracellular transport. To understand the flow of proteins, vesicles and organelles, we study the dynamics of tracers in complex environments, which are modeled using 1) a dense quasi-arrested matrix formed by colloidal hard spheres [1] and 2) a network of semi-flexible actin filaments. The dynamics of the tracer particles in both environments display an anomalous behavior. As a most striking feature the intermediate scattering function of the tracer particles dispersed in dense colloidal matrix displays an extended logarithmic decay resulting from the competition between localization and diffusion.

The characterization of tracer dynamics over a wide range of time and length scales relies on differential dynamic microscopy (DDM) [2-3], which is a powerful combination of microscopy and concepts of light scattering. Thanks to the recent successful extension of DDM to dense systems [4], the application to dense, crowded and multi-component biological systems is feasible.

[1] T. Sentjabrskaja et al., Nat. Com. 7 (2016). [2] R. Cerbino et al., Phys. Rev. Lett. 100 (2008). [3] F. Giavazzi et al., Phys. Rev. R 80 (2009). [4] T. Sentjabrskaja, PhD thesis, HHU (2015).