DY 51: Complex Fluids and Soft Matter - Part III (joint session DY/ CPP / BP)

Time: Thursday 15:00–16:45 Location: BH-N 334

Invited Talk DY 51.1 Thu 15:00 BH-N 334

Melting of soft disks: From liquid-hexatic coexistence to continuous transitions — •Sebastian C. Kapfer[1,2], Manon Michel[2], and Werner Krauth[2] — [1]Theoretische Physik 1, FAU Erlangen, Germany — [2]LPS, Ecole normale supérieure, Paris, France

The melting transition of two-dimensional solids has been a subject of continued research for more than fifty years, with the prevalent scenarios being the KTHNY theory of defect unbindung and a conventional first-order liquid-solid transition. For hard disks, the KTHNY scenario has recently been essentially confirmed, even though the liquid-hexatic step is of first order [1]. Using a new rejection-free global-balance Monte Carlo algorithm [2], we show that this result transfers to soft interactions with inverse power-law or Yukawa potentials [3]. The order of the liquid-hexatic step can be tuned from first-order to continuous by softening the potential. We show that there is always a hexatic phase separating the liquid and solid phases, and identify two regimes of the hexatic with vastly different correlation lengths. These results rationalize a plethora of simulation results obtained in the past, and could be verified in charged-colloid experiments.

[1] E. P. Bernard, W. Krauth, Phys. Rev. Lett. 107, 155704 (2011). [2] M. Michel, S. C. Kapfer and W. Krauth, JCP 140, 054116 (2014). [3] S. C. Kapfer, W. Krauth, preprint at arXiv:1406.7224.

DY 51.2 Thu 15:30 BH-N 334

Quasicrystalline Order and a "Crystal-Liquid" State in a Soft-Core Fluid — •Andrew Archer[1], Alastair Rucklidge[2], and Edgar Knobloch[3] — [1]Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK — [2]Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, UK — [3]Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA

Results will be presented for a two-dimensional system of soft particles interacting via a two-length-scale potential that may be considered to be a simple model for the effective interaction between dendrimers and other such polymeric macromolecules in solution. Density functional theory and Brownian dynamics simulations reveal the system has a fluid phase and two crystalline phases with different lattice spacing. Of these the larger lattice spacing phase can form an exotic periodic state with a sizeable fraction of highly mobile particles: a "crystal liquid". Near the transition between this phase and the smaller lattice spacing phase, quasicrystalline (QC) structures may be created by a competition between linear instability at one scale and nonlinear selection of the other. This dynamic mechanism for forming QCs is qualitatively different from mechanisms observed previously. The system first forms a small length scale crystal. Only when this phase is almost fully formed (i.e., the dynamics is far into the nonlinear regime) does the longer length scale start to appear, leading to the formation of QCs [A.J. Archer, A.M. Rucklidge, and E. Knobloch, Phys. Rev. Lett. **111**, 165501 (2013)].

DY 51.3 Thu 15:45 BH-N 334

A New Particle-Based Mesoscopic Model for Nematic Liquid Crystals — •Kuang-Wu Lee and Marco G. Mazza — Max-Planck-Institut für Dynamik und Selbstorganisation, 37077 Gottingen, Germany

We introduce a new mesoscopic model for nematic liquid crystals (LCs). This approach combines the particle-based stochastic rotation dynamics (SRD) method and the Ericksen-Leslie formulation of nematohydrodynamics. SRD has been used to investigate hydrodynamics at the mesoscopic level because it recovers the Navier-Stokes equation. We extend the SRD scheme to anisotropic fluids, i.e. nematic liquid crystals, by including the Ericksen-Leslie equations. We verify the applicability of this hybrid model by few study-cases in LC physics, e.g. the temperature-driven isotropic-nematic phase transition and the rheology of sheared LC. Our simulation results show that this hybrid model captures many essential aspects of LC physics at the macroscopic scale, while preserving microscopic thermal fluctuations.

DY 51.4 Thu 16:00 BH-N 334

Molecular simulations of liquid crystalline ferrofluids — •Stavros Peroukidis and Sabine Klapp — Institute of theoretical physics, Technical University of Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We explore the phase behavior and self assembly in binary mixtures of uniaxial rod and magnetic dipolar sphere particles by means of molecular simulations. We find that the mesogenic rods support the formation of orientational ordered ferromagnetic chains which, in turn, enhance the order of the liquid crystal. This ends up to liquid crystalline ferrofluids that possess two principal directors (one for each species). The antiparallel arrangement of the ferromagnetic chains, within the mesophases, cancels out macroscopic spontaneous magnetization. Depending on the relative size of the species, the directors are on average either parallel or perpendicular to each other, giving rise to uniaxial or biaxial liquid crystalline ferrofluids including: nematic, smectic, columnar phases and phase transformations between them.

DY 51.5 Thu 16:15 BH-N 334

Density functional theory for elongated polyhedra — •Matthieu Marechal and Klaus Mecke — Friedrich-Alexander-Universit\"at Erlangen-N\"urnberg

Due to recent advances in synthesis of nanoparticles and colloids, many-particle system of polyhedra are readily available for experiments. This has spurred a host of many-particle simulation studies on polyhedra. Recently, the lack of theoretical tools to study these system was amended by proposing a density functional theory (DFT) for polyhedra using the frame work of fundamental measure theory.

In this contribution, the application of DFT to elongated polyhedra will be discussed. Recent advancements in the DFT of long rods allow us to consider nematic and smectic liquid crystals in addition to the isotropic phase. We will consider these phases for triangular prisms that are elongated along their rotational symmetry axes. Colloids with this shape could be synthesized using nanolithography. We calculate the liquid crystal phase diagram and compare our results to Monte Carlo simulations.

DY 51.6 Thu 16:30 BH-N 334

Dynamical Crossover at the Liquid-Liquid Transformation of a Compressed Molten Alkali Metal — Taras Bryk[1,2], Simone De Panfilis[3,1], Federico A Gorelli[4,5], Eugene Gregoryanz[6], Michael Krisch[7], Giancarlo Ruocco[1,5], Mario Santoro[8], Tullio Scopigno[1,5], and •Ari Paavo Seitsonen[9,10] — [1]Dip. Fisica, Univ. La Sapienza, Roma, Italy — [2]Inst. Cond. Matter Phys. of NASU, Lviv, Ukraine — [3]Centre for Life Nano Science IIT@Sapienza, Istituto Italiano di Tecnologia, Roma, Italy — [4]Eur. Lab. for Non-Linear Spectr., Firenze, Italy — [5]IPCF-CNR, c/o Univ. La Sapienza, Italy — [6]Centre for Science at Extreme Conditions, Univ. Edinburgh, United Kingdom — [7]Eur. Synchr. Res. Facility, Grenoble, France — [8]IFAC-CNR, Sesto Fiorentino, Italy — [9]Dept. Chemie, Univ. Zürich, Switzerland — [10]Dépt. Chimie, ENS Paris, France

Density-driven phase transformations are a known phenomenon in liquids. Pressure-driven transitions from an open low-density to a higher-density close-packed structure were observed for a number of systems. Here, we show a less intuitive, inverse behavior. We investigated the electronic, atomic, and dynamic structures of liquid Rb along an isothermal line at 573 K, at 1.2-27.4 GPa, by means of ab initio molecular dynamics simulations and inelastic x-ray scattering experiments. Above 12.5 GPa, the breakdown of the nearly-free-electron model drives a transition of the pure liquid metal towards a less metallic, denser liquid, whose first coordination shell is less compact. Our study unveils the interplay between electronic, structural, and dynamic degrees of freedom along this liquid-liquid phase transition.