DY 53: Complex Fluids and Soft Matter (joint session DY/ CPP / BP)

Time: Wednesday 15:30–19:15 Location: BH-N 334

DY 53.1 Wed 15:30 BH-N 334

Tactoids and membranes of chiral rod-like particles — •Anja Kuhnhold and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Suspensions of chiral rod-like particles exhibit a rich phase diagram, including isotropic, chiral nematic (cholesteric) and smectic phases. The cholesteric phase is in particular shown by biological materials, such as fd viruses and cellulose nanocrystals [1].

Besides the bulk phases these rod-like particles assemble to objects of various geometries, e.g. tactoids (spindle-shaped droplets), twisted ribbons or colloidal membranes. Those assemblies are either found in the isotropic background phase of the same constituent particles or in mixtures with depletant particles [2]. Shape and structure of the resulting objects are determined by the interfacial tension with the surrounding phase and the elastic constants and chirality of the mesogens. Understanding the relation between molecular parameters, type (and strength) of interactions and final structures is needed to direct the 'engineering' of such systems to certain applications, e.g. sensing, templating.

We use Monte-Carlo simulations to study properties of tactoids and membranes composed of different (model) chiral rod-like particles. As depletants we use Asakura-Oosawa spheres. For the studied system sizes the tactoids are either nematic or smectic and the membranes appear as diverse twisted structures.

[1] J. Lagerwall et al., NPG Asia Materials **6**, e80 (2014).
[2] T. Gibaud, J. Phys.: Condens. Matter **29**, 493003 (2017).

DY 53.2 Wed 15:45 BH-N 334

The dynamics of smectic layer reorganization — •Patricia Dähmlow, Torsten Trittel, Kathrin May, Kirsten Harth, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

Centimeter-sized freely floating smectic bubbles are studied during their relaxation towards equilibrium spherical shape from an initial elongated hose-like one. These bubbles are observed via high-speed optical imaging. The film area of the nanometer thick bubbles decreases linearly with time within a few milliseconds, driven by capillary forces and inhibited by smectic layer reorganization. Compared to soap bubbles, this film area reduction is much slower, since the layer reorganization in smectics strongly dissipates energy.

Due to the surface reduction of the smectic bubble, the thickness of the film increases locally by forming ordered stacks of excess layers (islands). These islands grow until the equilibrium spherical bubble shape is reached. Additionally, we found, that the relaxation time of the bubbles depends on the film thickness. We discuss the limitations of a minimalistic model that captures smectic layer reorganization processes.

DY 53.3 Wed 16:00 BH-N 334

Mechanically induced smectic-C to smectic-A phase transition during the rupture of a thin film — •Torsten Trittel and Ralf Stannarius — Otto-von-Guericke Universität Magdeburg, 39106 Magdeburg, Germany

Mechanically induced phase transitions in condensed matter are quite rare, mostly they occur in the vicinity of the transition temperatures. We demonstrate a transition between liquid crystal mesophases that is induced far from the transition temperature, and involves solely capillary forces. The rupture of bubbles made from liquid crystal (LC) materials is observed with high speed imaging. In the smectic C phase, the LC molecules show a preferential tilt respective to the layers. We show that capillary forces during film rupture can trigger smectic C to smectic A transitions, which rapidly increase the film thickness while reducing the surface area of the films. The effect occurs on a microsecond scale, practically independent of film thickness and temperature.

DY 53.4 Wed 16:15 BH-N 334

Dynamics and rheology of ferronematics — •Gaurav P. Shrivastav and Sabine H.L. Klapp — Institut für Theoretische Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin.

Suspensions of magnetic nanoparticle (MNP) and liquid crystals (LC) show a rich variety of self-assembled structures and have a wide range of applications [1].

Using molecular dynamics (MD) simulations, we study the dynamical and rheological properties of these mixtures. We consider an 80:20 binary mixture of LCs and MNPs and perform MD simulations in NVT ensemble. We find that LC and MNP both show normal translational and rotational diffusive behavior in the isotropic and also in the nematic phase. However, in the nematic phase both species display an increased translational diffusion in the direction parallel to the nematic director.

To characterize the rheological properties of the mixture, we deform the bulk LC-MNP mixture by shearing it with constant shear rates. The stress-strain rate flow curve shows a shear thinning behavior in these mixtures. We also observe that the nematic order of LC and MNP both increases with strain but the degree of ordering in MNPs is higher than in LCs if the quiescent mixture is in the isotropic phase.

References:
[1] S. D. Peroukidis, and S. H. L. Klapp, Phys. Rev. E 92, 010501(R) (2015).
[2] G. P. Shrivastav, and S. H. L. Klapp, in preparation (2018).

DY 53.5 Wed 16:30 BH-N 334

Binary mixture thin film growth: A simulation study — •Eelco Empting, Miriam Klopotek, and Martin Oettel — Universiy of Tuebingen, Germany

We consider a binary lattice model for growth of demixing thin films. In addition to hard-core repulsion, the particles interact via attraction with their nearest neighbors, the strength of which depends on whether particles are of the like species. This system is a generalization of the regular solution theory model and can exhibit demixing and gas-liquid coexistence.

We present a spinodal decomposition diagram, which was obtained by mean-field calculations. We compare kinetic Monte Carlo simulations with expectations from this diagram. In general, deposition into spinodal regions of the phase diagram leads to demixing. With specific microscopic kinetics it is possible to arrest this demixing process. This leads to effects such as (i) kinetically limited demixing close to the surface and (ii) templated growth (repetition of the surface layer).

DY 53.6 Wed 16:45 BH-N 334

Confined Suspensions as Fluidic Hourglasses — Alvaro Marin[1], Henri Lhuissier[2], Massimiliano Rossi[3], and •Christian J. Kaehler[3] — [1]Physics of Fluids, University of Twente, The Netherlands — [2]IUSTI, Marseilles, France — [3]Bundeswehr University Munich, Germany

Objects of different nature are being forced through constrictions all the time: sand in an hourglass, particles in a fluid through a porous medium, blood through a narrowed vessel or people leaving a room in panic. In all these cases it is important to make sure that the system keeps continuously flowing, sometimes even lives are at risk. The case of particles in a fluid affects porous mediums, filters and membranes, which become unusable when clogged. We use microfluidic devices with a bottleneck of squared cross-section through which we force dilute polystyrene particle solutions with diameters comparable to the bottleneck size and down to one tenth its size. In low friction conditions and at certain opening sizes, we show experimental evidence of perfectly flowing particle system with no detectable clogging events even at its maximum concentration, just as it occurs in dry granular systems. We describe analytically such a transition by modelling the arch formation as a purely stochastic process, which yields a good agreement with the experimental data.

15 min. break

DY 53.7 Wed 17:15 BH-N 334

Phasonic equilibrium in colloidal quasicrystals — •Johannes Hielscher and Sebastian C. Kapfer — FAU Erlangen-Nürnberg, Institut für Theoretische Physik

We study decagonal intrinsic quasicrystals in two dimensions that are supported by a short-range double-minimum pair potential. Spatial correlations of phasonic flips [1], the preference of rational approximants at low temperatures [2], and energetic considerations indicate that a mathematically ideal quasicrystal is not an equilibrium state of this system.

We conduct Monte Carlo simulations of phasonic flips, using a model potential that separates configurational (phasonic) contributions from the influence of continuous (phononic) displacements. Amplitude and extent of collective phasonic excitations depend on temperature, hence also the frequencies of local motifs.

The isolation of the phasonic degrees of freedom enables a separate inspection of thermodynamic properties of these excitations, such as the heat capacity. We discuss how to translate these findings into the thermodynamics of systems governed by physical dynamics.

[1] J. Hielscher, M. Martinsons, M. Schmiedeberg & S. C. Kapfer: *J. Phys.: Cond. Matt.* **29**, 094002 (2017)

[2] A. Kiselev, M. Engel & H.-R. Trebin, *Phys. Rev. Lett.* **109**, 225502 (2012)

DY 53.8 Wed 17:30 BH-N 334

The delocalization transition in a colloidal glass — •Markus Gruber[1], Gustavo Abade[1], Matthias Fuchs[1], Antonio Puertas[2], Nesrin Senbil[3], and Frank Scheffold[3] — [1]U Konstanz, Germany — [2]U Almeria, Spain — [3]U Fribourg, Switzerland

Using microscopic probe particles we can study local transport processes and structural dynamics, especially of dense colloidal dispersions. In order to examine nonlinear phenomena such as shear melting, an external force has to be applied. We focus on the microscopic analogon of shear melting for the probe in a glassy host. The force on the probe is increased until it can break out of its cage and delocalize [1]. This phenomenon will be called the delocalization transition.

Our model system is a spherical probe particle subject to a constant external force in a colloidal suspension of hard spheres around the glass transition. The statistical dynamics of the probe particle can be expressed by the self-part of the van-Hove-function for the probe particles. We use a refined mode-coupling theory (MCT) approach for the self-intermediate scattering function for this calculation.

We find that the critical force is strongly connected to the strength of the local cages. Furthermore, the van-Hove-function exhibits an exponential tail in force direction, which increases in weight and correlation length when approaching the critical force. This indicates strong dynamical fluctuations, which will dominate measurements of active microrheology. These results are compared to molecular dynamics computer simulations as well as experiments on an emulsion glass.

[1] Gruber, Abade, Puertas, Fuchs, PRE 94, 042602 (2016)

DY 53.9 Wed 17:45 BH-N 334

Inhomogeneous bulk phases in fluids with competing interactions — •Daniel Stopper and Roland Roth — Institute for Theoretical Physics, University of Tuebingen, Germany

Using classical density functional theory, we theoretically study colloidal suspensions with so-called competing interactions, where in addition to a hard core interaction a short-ranged attractive force competes with a longer-ranged repulsive force. Remarkably, these kind of interactions can give rise to self-assembly into cluster phases without any external field. In particular, the clusters can form complex non-spherical three-dimensional periodically ordered structures [1,2]. For instance, it is found that the so-called Gyroid-phase can be thermodynamically stable - a structure which for instance is responsible for structural colors in specific types of birds or butterflies. Generally, besides the Gyroid-phase, several further types of structures can be stable including lamellar, cylindrical, or spherical micelles.

[1] Edelmann and Roth, Phys. Rev. E 93, 062146 (2016); [2] Stopper and Roth, Phys. Rev. E 96, 042607 (2017).

DY 53.10 Wed 18:00 BH-N 334

Squeezing bio-capsules into a constriction: deformation till break-up — •Badr Kaoui, Anne Le Goff, and Anne-Virginie Salsac — Biomechanics and Bioengineering Laboratory (UMR 7338), CNRS, Sorbonne Universités, Université de Technologie de Compiègne, Compiègne, France

We study experimentally the deformation and break-up of liquid-filled capsules trapped at an axisymmetric step constriction, and subjected to increasing pressure drops. We considered biological (trout fish eggs) and bioartificial (made of ovalbumin and alginate) ones, with the objective to characterize the transition to break-up. We find that both capsule populations behave as a brittle material. They do not exhibit any plastic deformation prior to break-up. Moreover critical pressure drop exhibits a stochastic behavior as known for the fracture of disordered media. The break-up probability follows a three-parameter Weibull distribution, from which one can deduce the capsule rupture characteristics [A. Le Goff, B. Kaoui, G. Kurzawa, B. Haszon, A.-V. Salsac, Squeezing bio-capsules into a constriction: deformation till break-up, Soft Matter 13, 7644 (2017)].

DY 53.11 Wed 18:15 BH-N 334

Screening in ionic liquids: an analytical approach — •Fabian Coupette and Andreas Härtel — University of Freiburg, Freiburg, Germany

Recent experiments report an unexpected increase of the electrostatic screening length in concentrated electrolytes [*Faraday Discuss.* **199**, 239 (2017)] which, as yet, lacks a theoretical foundation. The screening length can be obtained from the exponential long-range decay of the total correlation between ionic species, which in turn can be extracted from (classical) density functional theory. We propose a new functional for the primitive model of charged hard spheres which accounts for the packing of ions and solvent particles. With this approach, we find a universal behavior of the screening length in three distinct scaling regimes, including a strong increase at high ion concentrations. This increase culminates in a divergence of the screening length above a certain threshold. We validate our predictions by also performing Molecular Dynamics simulations, where we further observe a structural transition relatable to ion clustering close to the divergent regime. The universal scaling behavior matches well the experimental findings, however, differences remain which we will discuss in detail. We conclude that accounting for excluded volume is already inducing a strong increase in the screening length for concentrated systems, but insufficient to utter quantitative expectations for more intricate solvents, for instance polar ones. In this context we finally sketch the incorporation of dipolar interactions into our theory.

DY 53.12 Wed 18:30 BH-N 334

Charge-Scaling Effect on the Dynamics of an Ionic Liquid: A Molecular Dynamics Simulation Study — •Tamisra Pal and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt , Hochschulstraße 6, 64289 Darmstadt, Germany

We investigate the structural and dynamical relaxation processes in several charge-scaled 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][PF6]) room temperature ionic liquids (ILs) using molecular dynamics simulation, to quantify the relevance of the ionic charges on the temperature-dependent structural relaxation, including its dynamic heterogeneity. Charge-scaling provides an innovative way to systematically alter the dynamics of liquids by variation of a single control parameter. The rationale behind the use of reduced partial charges between ± 0.48 to 0.72 e is mainly governed by the charge-transfer mechanism taking place in the hydrogen bond between the imidazolium ring and the anion, along with the polarizability effects that invoked huge interest to better describe the dynamics in ILs. We perform extensive simulations from low temperatures in the viscous regime to high temperature far above the melting point to analyze the dependence of the dynamics on the ionic charges in a detailed manner. To characterize dynamics in terms of activation energies over the whole temperature range, recent studies on molecular glass formers have shown that E(T) can be split into low temperature cooperative energy $E_c(T)$ and high temperature constant activation energy E_∞. We extend these studies to relate the $E_c(T)$ associated with the collective molecular motion to the dynamical heterogeneity, e.g., to the size of clusters of mobile ions.

DY 53.13 Wed 18:45 BH-N 334

Hydrodynamics of droplet lattices in quasi 2D free-standing liquid crystal films — •Christoph Klopp, Torsten Trittel, Alexey Eremin, Kirsten Harth, and Ralf Stannarius — Otto-von-Guericke Universität Magdeburg

In an experiment on ISS, we prepared nearly regular triangular droplet lattices on free-standing liquid crystal films to investigate the diffusion and vibration dynamics on these lattices [1]. The layered structure in smectic A phases allows the preparation of thin and homogeneous macroscopic films. We record the motion of the droplets and calculate their diffusion characteristics. The experiments are compared to numerical simulations of droplet arrangements assuming specific repulsive interaction potentials. The mean-square displacement of the droplets reveals mobilities in the lattice and information on the strength of the potential.

The study was supported by NASA, DFG and DLR within the OASIS project.

[1] N. A. Clark, A. Eremin, M. A. Glaser, N. Hall, K. Harth, C.

Klopp, J. E. Maclennan, C. S. Park, R. Stannarius, P. Tin, W. N. Thurmes, and T. Trittel, Realization of hydrodynamic experiments on quasi-2D liquid crystal films in microgravity, ASR Volume 60, 737-751, 2017

DY 53.14 Wed 19:00 BH-N 334

ROLE OF PORE FORMING TOXINS IN MODULATING THE LIPID DYNAMICS. — •Vadhana Varadarajan[1], Rajat Desikan[2], and Ayappa Ganapathy K[3] — [1]Indian Institute of Science, Bangalore, India — [2]Indian Institute of Science, Bangalore, India — [3]Indian Institute of Science, Bangalore, India

Pore-forming toxins (PFT's) secreted by bacteria are important bacterial virulence factors which oligomerize and spontaneously self-assemble on the mammalian cell membranes. The effect of an alpha PFT and a beta-PFT on saturated and unsaturated mammalian cell membranes are investigated using molecular dynamics simulations. The structure and dynamics of lipids in the vicinity of PFT's are different away from them giving rise to structural and dynamic heterogeneities. We also investigated the role of cholesterol in these systems. Our findings reveal that cholesterol fluidizes the lipid bilayer and the local structure is closely related to the dynamics which also depends on the saturation level of the lipid as well as the hydrophobic mismatch of the lipid bilayer with the PFT's. We also investigated the survival probability of the lipids in the vicinity of PFT which can be used to quantify the lifetime and death of cells. Our study reveals that the beta-PFT is less toxic than alpha-PFT.