DY 54: Poster: Complex, Fluids, Glasses, Granular

Time: Thursday 15:00–18:00 Location: Poster B2

DY 54.1 Thu 15:00 Poster B2

A Phase Field Crystal Approach for Patchy Colloids — •Robert F. B. Weigel and Michael Schmiedeberg — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany

Patchy colloids are particles with discrete rotational symmetry and anisotropic interaction, thus preferring certain bond angles. Finding the complex equilibrium phases in systems with patchy colloids is challenging.

We propose and study a mean field model for patchy colloids that is motivated by the phase field crystal theory for systems with particles exhibiting 2-fold rotational symmetry as in liquid crystals for which a theory has been proposed in [1]. In such an approach the free energy $F[\psi, U]$ is given as a functional of a real-valued density-like field ψ and a complex-valued orientation field U, which encodes the intensity and direction of the orientation. As usual in phase field crystal models, F is composed of a Landau-like power series in the fields along with an expansion with respect to the gradients as well as coupling terms respecting the rotational symmetry of the particles. Numerical minimization of F yields a rich phase diagram of complex structures. Our special interest is to find out how orderings with non-crystallographic symmetries, such as in quasicrystals, can be obtained.

[1] Achim *et al.*, Phys. Rev. E **83**, 061712 (2011)

DY 54.2 Thu 15:00 Poster B2

X-ray Particle Tracking of Granular Materials — •Luis Torres-Cisneros[1], Kit Windows-Yule[2], Patric Müller[1], and Thorsten Pöschel[1] — [1]Institute for Multiscale Simulation, Cluster of Excellence "Engineering of Advanced Materials", Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Deutschland — [2]School of Physics and Astronomy, University of Birmingham, Edgbaston, United Kingdom

Nowadays the fundamental understanding of granular materials (a finite amount of macroscopic fragmented matter that interacts mainly by dissipative collisions and friction) flowing is one of the most exciting challenges. We could find these systems present in nature as in industry; i. e., in a rock avalanche or in silo downloading corn grains. Given that there are in the literature many theoretical studies done in order to understand its underlying rules an experimental setup capable to corroborate it is needed.

In the last years the X-ray tomography appeared to let us able to have an insight in granular materials at static conditions, as a non-invasive technique. But given that we could find a granular system in a fluid-like state the present tools used to study granular materials at static conditions are not suitable. In this way the present research is aimed in order to establish the main ideas concerning the features needed in an X-Ray machine capable to track the trajectories in a granular system at non-static conditions.

DY 54.3 Thu 15:00 Poster B2

Rheology of a model composite of liquid crystals and magnetic nanoparticles — •Nima H. Siboni, Gaurav P. Shrivastav, and Sabine H. L . Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36 D-10623 Berlin

Liquid crystals (LC) functionalized with nano-to-micro sized magnetic particles (MNP) have attracted much recent attention due to their rich self-assembly, dynamics and a wide range of applications [1]. Using molecular dynamics (MD) simulations, we show that the flow properties of the LC matrix can be modified by the inclusion of spherical MNPs.

We study the rheology of an 80:20 binary mixture of LCs and MNPs in the isotropic phase for various dipolar coupling strengths of the MNP by shearing it via Lees-Edwards periodic boundary conditions with constant shear rates. The mixture shows a shear thinning behavior for the considered range of the dipolar coupling strength. The extent of the non-Newtonian region in the flow curve increases with increasing dipolar coupling strength of the MNPs. The nematic order in LC and MNP both increases with strain, however, the degree of ordering in MNPs is higher than in LCs.

References:

[1] G. P. Shrivastav, and S. H. L. Klapp, arXiv:1809.08288 (2018).

[2] G. P. Shrivastav, N. H. Siboni and S. H. L. Klapp, in preparation.

DY 54.4 Thu 15:00 Poster B2

Investigation of the glassy dynamics of charged Lennard-Jones systems with molecular dynamics simulations — •Lukas Hecht, Robin Horstmann, and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, Hochschulstraße 6, 64289 Darmstadt, Germany

The explanation of the glass transition is one of the most challenging topics in physics of condensed matter. To get ahead, recent work investigated systematically altered water and silica variants in bulk and confinement to ascertain the glass transition behavior via molecular dynamics simulations [1]. A strong relation between the activation energy in the simple liquid regime at high temperatures and the glass transition temperature was found. Moreover, it proved useful to decompose the activation energy into a temperature independent part and a temperature dependent part associated with cooperative dynamics, which is an exponential function of temperature [2].

Since water and silica have a complex structure with prefered order, it is difficult to ascertain basic mechanisms behind the glass transition. Therefore, we focus on simpler systems, explicitly mixtures of charged Lennard-Jones atoms. We vary the mixing ratio of the atoms as well as their partial charges and analyze their dynamics in wide temperature ranges. In this way, it is possible to strongly vary the high-temperature activation energy and the glass transition temperature and, thus, to obtain further insights into their relation.

[1] J. Geske et al., Z. Phys. Chem., 2018, 232(7-8), pp 1187-1225

[2] B. Schmidtke et al., Phys. Rev. E, 2012, 86, 041507

DY 54.5 Thu 15:00 Poster B2

Thermodynamic bond-angular instability drives glass formation — •Andrii Babich[1,2], Maria Göbel[1,5], Volodymyr Bugaev[2,3], Johannes Roth[3], Gerhard Grübel[1,4], and Peter Wochner[2] — [1]Center for Ultrafast Imaging,University of Hamburg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Institute for Functional Matter and Quantum Technologies, University of Stuttgart — [4]DESY, Hamburg — [5]Max Planck Institute for Intelligent Systems, Stuttgart

Glasses are indispensable in everyday life and technology. However, the microscopic mechanisms generating this state of matter remain subject to debate. Within MD simulations and the original statistical-thermodynamic ring approximation, we revealed that at the vitrification the 4-point positional correlations caused by the configurational entropy create an instability with respect to formation of a structural state with angular order. This state is described in terms of only one dominant orientational mode in the angular statistical variance of the density fluctuations, which results in a mesoscopic-scale mutual ordering of the polytetrahedral clusters. Their lifetime exhibits the well-known slowdown at approaching the glass transition point. Our results can be tested by coherent diffraction experiments at the newly developed light sources and will be an essential guide to determine the best conditions for successful experiments in a broad range of glassy systems, e.g. colloidal, metallic glasses and water.

DY 54.6 Thu 15:00 Poster B2

The Quest for Spontaneous Core Rotation in Ferrofluid Pipe Flow — •Max Fabian Steudel, Ingo Rehberg, and Reinhard Richter — Experimentalphysik 5, Universität Bayreuth, Bayreuth, Germany

Ferrofluidic pipe flow in a constant [1] or alternating [2] axial magnetic field has attracted much interest because the flow can conveniently be controlled by the parameters of the applied field. More recently, for a flow in a static field, a transition from a purely axial flow to a steady swirling one has been unveiled in analytical and numerical studies [3]. The swirl appearance is predicted to yield a sharp increase of the flow rate [3]. To uncover this transition we measure the flow rate of different types of ferrofluid as a function of the applied magnetic field.

[1] M. A. Martsenyuk, Y.L. Raikher and M. I. Shliomis, Sov. Phys. JETP **38**, 413 (1994).

[2] A. Zeuner, R. Richter and I. Rehberg, Phys. Rev. E **58**, 6287 (1998).

[3] Alexei Krekhov and Mark Shliomis, Phys. Rev. Lett. **118**, 114503 (2017).

DY 54.7 Thu 15:00 Poster B2

Structural and mechanical properties of sodium, magnesium, and calcium metaphosphate glasses: insights from molecular dynamics simulations — •Achraf Atila and Erik Bitzek — Materials Science & Engineering, Institute I, Friedrich-Alexander Universität Erlangen-Nürnberg (FAU)

Phosphate glasses are of great interest in various industrial, technological and clinical applications. Compared to silicate glasses, they have a lower glass transition and melting temperatures. Doping phosphate glasses by alkali or alkaline earth ions reduces the glass transition temperature and makes them more chemically durable. Metaphosphate glasses, defined as the composition in which the ratio O/P is three, have a chain-like structure made of PO_4 tetrahedra. These glasses are usually isotropic due to the random orientation of the chains. Until now, there are few atomistic simulations studies on the mechanical and structural properties of binary metaphosphate glasses. Here, we present molecular dynamics simulations regarding the effect of different non-framework cations (Na^+, Ca^{2+}, Mg^{2+}) on the structural and the mechanical properties of the metaphosphate glasses using a Morse-type pair potential with Coulomb interactions (J. Phys. Chem. B, 2006, 110 (24), pp 11780−11795). We investigate and compare the mechanical properties of these glasses by applying tension, compression, and shear. Radial distribution functions, their projections on spherical harmonics and angular distribution functions are used for analyzing the glasses structure.

DY 54.8 Thu 15:00 Poster B2

Molecular dynamics study of structural and dynamic properties of ionic liquids at amorphous silica surfaces — •Robin Koester, Tamisra Pal, and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

Structural and dynamic properties of imidazolium-based ionic liquids change severely in presence of rigid interfaces. Previous molecular dynamics studies of [Bmim][NTf_2] revealed layered structures and a considerable slowdown of dynamics in the layers next to amorphous silica surfaces [1]. In recent simulation studies of [Bmim][PF_6] and [Bmim][BF_4] similar effects for systems confined by amorphous silica slit pores were found [2]. For both anions preferential localization at irregularly distributed sites at the interface can be observed. While these sites differ in volume and number of associated silanol groups, favourable local structures appear to be a major determinant. Building on the preceding studies, we relate the residence time to the structural properties of the silica surface near the adsorption sites to obtain a microscopic understanding for the mechanism of the slowdown in the interfacial layer. Additionally, we examine anion dynamics by means of spatially resolved analysis of correlation functions. Further investigations aiming for a better understanding of the slowed down dynamics involve the examination of anion dynamics in terms of hopping motion required to change site.

[1] Li et al., Langmuir, 2013, 29, pp. 9744-9749
[2] T. Pal and M. Vogel, J. Phys. Chem. C, 2018, 122, pp. 624-634

DY 54.9 Thu 15:00 Poster B2

Electrohydrodynamic instabilities of droplets suspended in highly viscous liquids — Sebastian Rühle, •Martin Brinkmann, and Ralf Seemann — Experimental Physics, Saarland University

Motivated by recent experimental results we study electroconvective flows in poorly conducting droplets that are suspended in an ambient liquid with high viscosity and conductivity. The coupled electrostatic and Stokes problem for a homogeneous external field is solved numerically for both 2d and axially symmetric 3d droplets using a boundary element approach. A number of dynamical flow regimes and instabilities are observed whose appearance is controlled by the contrast of viscosity, conductivity, and dielectric permittivity, as well as the magnitude of the applied field. If the timescale of charging or discharging of the 2d droplets is comparable or larger than the timescale of flow, the droplets may display transient shape oscillations and rotational flows.

DY 54.10 Thu 15:00 Poster B2

Fast calculation method for determining the shape of static liquid/liquid or liquid/vapor interfaces under the influence of electrical fields — •Sebastian Bohm and Erich Runge — Technische Universität Ilmenau, FG. Theoretische Physik 1, Weimarer Straße 25, 98693 Ilmenau

Due to the constant trend towards smaller systems new methods for the manipulation of liquids on the micro-scale are required. One important and frequently used technique to manipulate liquids on small scales is the so called Electrowetting-on-Dielectrics (EWOD) effect. EWOD based microfluidic devices provide high-throughput platforms for a wide range of applications in biology, chemistry and nanotechnology. For the design and optimization of such devices, the shape of liquid/vapor or liquid/liquid interfaces needs to be determined. However, the numerical simulation presents a great challenge due to the coupling of fluidics and electrodynamics.

This work reports a new and fast method for the determination of the shape of static three-dimensional interfaces under the influence of electrical fields. Additionally, the influence of interface effects and gravity are considered. The simulation also allows to determine the shape of the interface near the contact line with high accuracy and verify that the local contact angle at the contact line is voltage independent. The simulation results are confirmed by EWOD experiments on systems with different geometries.

DY 54.11 Thu 15:00 Poster B2

Self-assembly in magnetic filament systems: impact of internal factors — •Elena Pyanzina, Tatjana Belyaeva, Marina Kashpurova, and Ekaterina Novak — Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia

The fundamental understanding of the self-assembly properties of colloidal systems is one of the key topics in current research on novel microstructured soft materials and technologies. In this work we investigate self-assembly of magnetic filaments of different topology with different additional interaction and particles polydispersity. We performed molecular dynamics simulations using a Langevin thermostat. Cluster analysis based on graph theory is used to analyze the obtained data. At the moment we are analyzing the results, but we can already say that the introduction of additional attraction and particles polydispersity significantly expands the structural diversity of the self-assembly of magnetic filaments, and the effect of magnetic dipole-dipole interaction remains substantial. All these results will pave the way for the development of analytical models and identify the most interesting building block candidates for the design of new magnetoresponsive materials.