Berlin 2015 – DY Monday

DY 5: Colloids and Complex Liquids I (joint session CPP/ BP/ DY)

Time: Monday 9:30–12:45 Location: C 130

DY 5.1 Mon 9:30 C 130

Disclination lines at homogeneous and heterogeneous colloids immersed in a chiral liquid crystal — $\bullet {\sf SERGEJ}$ SCHLOTTHAUER¹, MICHAEL MELLE¹, CAROL K. HALL², ENRIQUE DIAZ-HERRERA³, and MARTIN SCHEON¹.² — ¹Technische Universität Berlin, Berlin, Germany — ²North Carolina State University, Raleigh (NC), USA — ³Universidad Autonoma Metropolitana-Iztapalapa, Iztapalapa , Mexico

We perform Monte Carlo simulations in the isothermal-isobaric ensemble to study defect topologies formed in a cholesteric liquid crystal due to the presence of a spherical colloidal particle. Topological defects arise because of the competition between anchoring at the colloidal surface and the local director. We consider homogeneous colloids with either local homeotropic or planar anchoring to validate our model by comparison with earlier lattice Boltzmann studies. The presence of a Janus colloid in a choleteric host fluid reveals a rich variety of defect structures. Using the Frank free energy we analyze these defects quantitatively indicating a preferred orientation of the Janus colloid relative to the cholesteric helix.

DY 5.2 Mon 9:45 C 130

Anisometry versus anisotropy in systems of colloidal magnetic cubes — $\bullet {\tt Joe}$ Donaldson¹ and Sofia Kantorovich¹.² — ${\tt ^1Faculty}$ of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — ${\tt ^2Ural}$ Federal University, Lenin av. 51, 620083, Ekaterinburg, Russia

Contemporary colloid science provides numerous ways of synthesising particles with non-spherical geometries. Indeed, a whole spectrum of shapes is now readily accessible, cubes being one such example. The directionally dependent interactions of these particles are key tools in the development of new soft materials. An additional internal anisotropy is introduced into the system when these particles are constructed from a magnetic medium. Consequently, the interplay between anisometry and anisotropy, and its influence on how magnetic particles self-assemble, can be studied. Two different magnetic orientations within the cube have been considered; the first is represented by a dipole aligned along the [001] crystallographic axis, and the second by a dipole aligned along the [111] axis. We have determined the ground state structure of isolated clusters for both systems and have shown for the [001] orientation a preference for a ground state dominated by chain formation. In contrast, clusters of [111] orientated particles tend to arrange in lattices within which dipoles form ring structures consisting of four dipoles. We shall discuss the consequences of these structural configurations on the bulk properties of such systems, including preliminary predictions of the magnetic properties of dilute suspensions.

DY 5.3 Mon 10:00 C 130

Active microrheology of a nematic Liquid crystal — •TILLMANN STIEGER 1 , ANDRÉS CÓRDOBA 2 , MARCO G. MAZZA 3 , JUAN J. DE PABLO 2 , and MARTIN SCHOEN 1 — 1 Technische Universität Berlin — 2 University of Chicago — 3 MPIDS Göttingen

The knowledge of rheological properties of soft matter is of great importance for a variety of applications such as lubricants or the reduction of friction. The rheology of materials becomes particularly relevant if systems are miniaturized to the nanometer length scale at which physical properties of soft matter are altered significantly from their microscopic bulk properties. The focus of this work are nematic liquid crystals (LC) which are characterized by a high degree of orientational order along a specific direction. If now a colloid is immersed into such a nematic host phase properties of the later are effected greatly at the nanoscale. The colloid perturbs orientational order of the nematic LC in its vicinity. This causes defect topologies to arise. We present nonequilibrium molecular dynamics (MD) simulations of a homogenous colloid with either planar or perpendicular anchoring of LC molecules at the colloid's surface. This leads to well known defect topologies such as the Boojum defect or the Saturn ring. The colloid is moved periodically, comparable to a typical experimental setup where one uses optical tweezers. The phase shift and the magnitude of the measured force response is used to investigate viscoelastic properties of the LC host phase. Specifically, we are interested in calculating the dynamic modulus G=G'+iG'', where G' and G'' are storage and

loss moduli. For both quantities we present analytic expressions that can be used to analyse our MD data.

DY 5.4 Mon 10:15 C 130

Characterizing Dissipation during the Crystallization Process
— •Sven Dorosz — 162a avenue de la faiencerie, L1511 Luxemburg

I present computational results on the compression of a hard sphere liquid into the solid phase in finite time.

I will discuss the properties of the resulting work distributions and in particular focus on the correlations between the dissipated heat during the process and the detected structures in the solid resp. melt.

DY 5.5 Mon 10:30 C 130

Colloidal Plastic Crystals of Hard Dumbbells under Shear — •NILS HEPTNER^{1,2}, FANGFANG CHU^{1,2}, MATTHIAS BALLAUFF^{1,2}, and JOACHIM DZUBIELLA^{1,2} — ¹Helmholtz-Zentrum Berlin, Germany — ²Humboldt-Universität zu Berlin, Germany

We study the structural response of plastic crystals of colloidal dumbbells to an oscillatory shear field using Brownian Dynamics (BD) computer simulations. Under increasing shear strains, a discontinuous transition is found from a twinned-fcc like crystal to a partially oriented highly ordered sliding-layer state via a disordered intermediate state. In this novel partially oriented sliding-layer phase, sheared hard dumbbells exhibit a small but finite collective orientational order. We show that the orientations of only weakly anisotropic particles play a crucial role in non-equilibrium transitions. Our findings from simulations are compared to data obtained by rheo-SANS experiments and reveal the nature of a second rheological yielding event which has not been observed for crystalline suspensions of hard spheres.

DY 5.6 Mon 10:45 C 130

Experimental determination of structural and dynamical heterogeneities in a metastable colloidal fluid — Sebastian Golde¹, Markus Franke², Thomas Palberg³, and •Hans Joachim Schöpe⁴ — ¹Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — ²DB Systel GmbH, Weilburger Straße 22 B4.14, 60326 Frankfurt a. Main — ³Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — ⁴Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

Metastable fluids exhibit heterogeneous dynamics as well as heterogeneous structure [1]. These dynamical and structural heterogeneities play an important role in the understanding of the glass transition and crystallization. Simulations suggest that these heterogeneities in dynamics and structure are linked, but the direct experimental proof is still lacking [2]. Using space- and time-resolved dynamic light scattering and time-resolved multi angle static light scattering [3], we study the dynamics and structure in a model system of colloidal hard spheres during crystallization and vitrification. For the first time, direct correlation between the temporal evolution of the dynamical heterogeneities and the structural heterogeneities was obtained from an analysis of the subensemble resolved particle dynamics and the evolution of the static structure factor.

[1] L. Berthier and G. Biroli, Rev.s of Mod. Phys., 83, (2011,[2] T. Kawasaki and H. Tanaka, JPCM, 22 (2010),[3] M. Franke, S. Golde and H.J. Schöpe, Soft Matter 10, 5380 (2014)

15 min. break

DY 5.7 Mon 11:15 C 130

Dense Colloidal Suspensions in Microfluidic Flow — ●PHILIPP KANEHL and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Dense colloidal suspensions in a pressure driven flow accumulate in the center of the microchannel. Bidisperse mixtures partially demix depending on their densities [1]. In very dense colloidal systems, one observes oscillations in the colloidal flow velocity which is attributed to transient jamming. The oscillations ultimately become irregular when density is further increased [2].

To develop a theoretical understanding of all these effects, we simulate hard spheres under pressure-driven flow in two and three dimensions using the mesoscale simulation technique of multi-particle colli-

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sion dynamics which is an efficient solver of the Navier-Stokes equation and includes thermal motion.

In our simulations, we reproduce the experimental observations that a monodisperse suspension enriches the channel center and a binary mixture segregates into its two species. Comparison with our analytical model suggests that Brownian motion is crucial for demixing and that the non-diagonal elements of the collective diffusion tensor determines, which species enriches the center. Qualitative differences between 2 and 3 dimensions are found.

Finally, we present first results on monodisperse suspensions near close packing to understand flow oscillations and transient jamming.

- [1] D. Semwogererea and E. R. Weeks, Phys. Fluids, 20, (2008).
- [2] A. I. Campbell and M. D. Haw, Soft Matter 6, (2010).

DY 5.8 Mon 11:30 C 130

Rheological study of anisometric pigment particle suspensions — •Yong Geng, Alexey Eremin, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg, FNW/IEP/ANP, Postfach 4120, 39016 Magdeburg, Germany

Rheological properties of colloidal suspensions formed by nanometer size rod-shaped pigment particles dispersed in a non-polar solvent are studied. Experiments have shown that these suspensions possess unusual properties such as liquid crystalline behaviour at high dispersant concentration, field-induced phase separation at low and intermediate concentrations, switching in electric fields, and a reversible response to the adsorbing light affecting current transients in sandwich cells.1 By doping with small amounts of ferrofluid these pigment dispersions can form a basis for magneto-responsive materials. A strong magnetooptical effect has been confirmed. In our studies, we demonstrate a strong shear-induced birefringence and shear thinning behaviour in pure dispersions. We also discuss the effects of magnetic fields on the rheological properties of the pigment/ferrofluid mixtures. This helped to get a deeper insight into the properties of these suspensions and understand the mechanisms of the structural changes under external field such as electric, magnetic and flow.

 $1.\ \,$ Eremin, Alexey, et al., Adv. Funct. Materials 21.3 (2011): 556-564.

DY 5.9 Mon 11:45 C 130

Structure analysis of stable and metastable hard sphere fluids by confocal microscopy — Achim Lederer¹ and •Hans Joachim Schöpe² — ¹Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — ²Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

The structural properties of the metastable melt play a key role in the understanding of the glass transition and crystal nucleation. Using laser scanning confocal microscopy we study the structure of stable and metastable colloidal hard sphere fluids. The used system was characterized with extreme care to allow a meaningful comparison with theory and simulation. While the Percus-Yevick (PY) approximation works quite perfectly for stable fluids at moderate volume fractions, it starts to fail for volume fractions larger than 0.45 approaching the freezing transition at 0.494. Strong deviation can be observed in metastable fluids: In the pair correlation function g(r) the experimental data display a significant higher principal peak and a different shape in the higher order peaks than the PY-approximation. In the static structure factor S(q) the data display a split in the second

structure factor maximum suggesting a local short range crystalline like order. An analysis on the particle level reveals the existence of clusters with higher bond orientation order (q6(i)q6*(j)), although the overall hexagonal order of the ensemble does not increase.

DY 5.10 Mon 12:00 C 130

Effects of shear and walls on the diffusion of colloids in microchannels — •SOMNATH GHOSH, FRIEDER MUGELE, and MICHEL DUITS — Physics of Complex Fluids group, MESA+ institute, University of Twente PO Box 217, 7500 AE Enschede, The Netherlands

Colloidal suspensions flowing through micro-channels were studied for the effects of both shear flow and the proximity of walls on the particles* self-diffusion. Use of hydrostatic pressure to pump micron-sized silica spheres dispersed in water-glycerol through poly (dimethylsiloxane) channels with a cross section of 30x24 micron, allowed variation of the Péclet number (Pé) from 0.01 to 50. To obtain diffusion coefficients, image-time series from a Confocal Scanning Laser Microscope were analysed with a method that, after finding the particle trajectories, subtracts the instantaneous convective displacements and subsequently measures the slopes of the Mean Squared Displacement in the flow (x) and shear (y) directions. The thus obtained Dx and Dy, which should be equal to the free diffusion coefficient (regardless of shear) in the dilute limit, both increase strongly with Péclet number (for Pé>10) in a concentrated suspension. This effect of shear-induced collisions is counteracted by the contribution of walls, which cause a strong local reduction in Dx and Dy.

DY 5.11 Mon 12:15 C 130

Transport of active particles in low-porosity structures — Frank Wirner¹, Christian Scholz¹, and •Clemens Bechinger^{1,2} — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Transport of active bacteria in porous media is of importance in many different fields, ranging from bioremediation, groundwater contamination and enhanced oil recovery to blood perfusion inside the body. We study the motion of active particles in artificially created porous media by a semi-experimental approach. In porous media with low porosities the presence of stagnant parts can lead to a temporary trapping of active particles in such regions, which can vastly increase their retention times. We compare the distributions of retention times and the transport properties of active and purely Brownian particles.

DY 5.12 Mon 12:30 C 130

Isobutyric acid and water mixture confined in a silica nanopore — • MICHAEL HARRACH and BARBARA DROSSEL — Institut für Festkörperphysik, TU Darmstadt, Darmstadt, Germany

We analyze the phase behaviour of water and isobutyric acid mixtures of differing weight percentages, in a silica nanopore of roughly 4 nm diameter and a corresponding smooth-walled confinement based on the average potential as given by the pore. While experimental studies have been interpreted as showing evidence for a phase seperation of water and isobutyric acid with the water situated at the pore wall we observe the converse, with the water rich part of the mixture preferring the pore center. The comparison of the smooth and rough pore allows us to further determine the importance of potential hydrogen bond sites and their influence on the static and dynamic characteristics of the mixture.