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

Time: Wednesday 15:00–19:15   Location: H3

Invited Talk   CPP 47.1   Wed 15:00   H3
Phase-separation in an elastic matrix: from living cells to synthetic materials — •Eric Dufresne — ETHZ

In order to function effectively, living cells need to compartmentalize myriad chemical reactions. In the classic view, distinct functional volumes are separated by thin oily-barriers called membranes. Recently, the spontaneous sorting of cellular components into membraneless liquid-like domains has been appreciated as an alternate route to compartmentalization.

I will review the essential physical concepts underlying these phenomena and outline some of the fundamental questions in soft matter physics that they inspire. Then, I will describe our recent experiments exploring the impact of mechanical stresses on the condensation of droplets. This work spans experiments with living cells and synthetic polymer networks, with an eye toward useful new materials.

CPP 47.2   Wed 15:30   H3
Breakup of a particulate suspension jet — •Joris Chateau[1,2] and Henri Lhuissier[1] — [1]CNRS, Aix-Marseille University, Marseille, France — [2]Max Planck Institute, Gottingen, Germany

As viscosity is increased, a liquid capillary jet accelerated by gravity stretches over increasingly large distances before eventually breaking up. This Newtonian behavior is profoundly altered for particulate suspensions. Adding solid particles to a liquid, which increases the effective viscosity, can paradoxically shorten the jet considerably. This apparent contradiction is rationalized by considering finite size effects occurring at the scale of a few particles. A model is presented which captures the breakup length of suspension jets observed experimentally for a broad range of liquid viscosities, particle sizes and extrusion velocities of the jet, and recovers the Newtonian case for vanishing particle sizes. These results can be readily extended to any stretched jet configuration and potentially to other fluid media having a granularity.

CPP 47.3   Wed 15:45   H3
Self-assembly and dynamics of mixtures of magnetic and non-magnetic liquid crystals under shear and external magnetic field — •Nima H. Siboni, Gaurav P. Shrivastav, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36 D-10623 Berlin

Doping liquid crystals with magnetic particles of different shapes enables us to control the properties of this delicate phase of matter via an external magnetic field [1,2]. In this talk, we focus on mixtures where the magnetic particles have the same shape as the liquid crystals. We study the self-assembly and dynamics of the mixture in and out of equilibrium [3]. In particular, we utilize non-equilibrium molecular dynamics simulation of Gay-Berne particles [4] to study (i) the (composition-dependent) effect of an external magnetic field on the isotropic-to-nematic transition of the mixture, and (ii) the interplay between shear-induced order and the magnetic field-induced order on the mechanical response of the mixture to an applied external shear.

References:

[1] I. Dierking, and S. E . San, Appl. Phys. Lett. **87**, 233507 (2005).
[2] G. P. Shrivastav, and S. H. L. Klapp, arXiv:1809.08288.
[3] N. H. Siboni, G. P. Shrivastav, and S. H. L. Klapp, *in preparation*.
[4] J. G. Gay, and B. J. Berne, J. Chem. Phys., **74**, 3316 (1981).

CPP 47.4   Wed 16:00   H3
Marangoni flow in thin freely suspended liquid films — •Torsten Trittel[1], Christoph Klopp[1], Kirsten Harth[2], Alexey Eremin[1], and Ralf Stannarius[1] — [1]Institute for Physics, Otto von Guericke University, 39106 Magdeburg — [2]Physics of Fluids and Max Planck Center for Complex Fluid Dynamics, P.O. Box 217, 7500 AE Enschede

Next to their great success in display applications, liquid crystals are enormously attractive in the field of fundamental physics. Freestanding films with unique aspect ratios can serve as an ideal system for the investigation of two-dimensional hydrodynamics. We focus on thermocapillary effects in such films under microgravity. We present results of two suborbital rocket flights and show that thermal gradients within the film plane can cause thermocapillary (Marangoni) effects. The temperature dependence of the surface tension $\sigma(T)$ can induce flow from the hot to the cold film edge. Finally we developed a hydrodynamic model that can describe the experimental observations quantitatively. In contrast to Benard-Marangoni or Rayleigh-Benard convection, the relevant control parameter is the temperature difference, not the temperature gradient across the film.

CPP 47.5   Wed 16:15   H3
Shear-waves from cavitation in soft solids — •Julien Rapet[1,2], Yoshiyuki Tagawa[3], and Claus-Dieter Ohl[1,2] — [1]Nanyang Technological University, Singapore — [2]Otto-Von-Guerricke Universität, Magdeburg, Germany — [3]Tokyo University of Agriculture and Technology, Tokyo, Japan

While the fluid mechanics of cavitation is a mature research area, very little is known for bubbles undergoing large and non-spherical volume changes in a soft elastic solid. Here soft solids made from gelatin-water mixtures mimic tissue. Previous studies demonstrated that the collapse of a bubble entrapped in soft solids emits longitudinal waves at the speed of sound. Yet the elasticity of the medium supports also transversal waves propagating at a considerable lower speed. We show how cavitation in elastic solids may lead to the emission of such shear waves, particularly the collapse of bubbles near an air/solid interface. The cavitation bubbles are obtained by focusing a pulsed laser into the tissue mimicking material. The bubble dynamics and shear wave propagation are observed with high-speed imaging and photoelastic imaging, respectively. We show that similar to water the cavity moves during collapse away from the free surface accelerating a jet in the direction of the bubble's center of mass motion. During this process the volume between the air/solid interface and the bubble is sheared. Yet the dynamics is much faster than the shear wave speed and therefore the shear stress remains confined. For sufficiently strong and non-spherical collapses, the gelatin surface deforms and a crack starting from the interface propagating towards the bubble.

CPP 47.6   Wed 16:30   H3
Self-organized lattices and coalescence of droplets in freely suspended liquid crystal films — •Christoph Klopp[1], Torsten Trittel[1], Kirsten Harth[2], Alexey Eremin[1], and Ralf Stannarius[1] — [1]Otto von Guericke University, Institute for Physics, 39106 Magdeburg, Germany — [2]Universiteit Twente, Physics of Fluids and Max Planck Center for Complex Fluid Dynamics, 7500 AE Enschede, The Netherlands

Colloids in freely suspended smectic films are an excellent system to study self-organisation in restricted (2D) dimensionality. The dynamics of the colloids in such films is fully 2D. We demonstrate the formation of two-dimensional hexagonal lattices of isotropic droplets stabilized by repulsive interactions in freely suspended films [1]. The dynamics of single droplets in a six-neighbor cage can be described using the Saffman model for mobility in a 2D fluid. We show that the modified model reproduces the experimental observations, the droplet mobility in the lattice depends only on the ratio of cage and droplet sizes, irrespective of droplet sizes. At higher temperatures, droplets coalesce. Droplets on free-standing films have the shapes of flat lentils and their coalescence dynamics are expected to be intermediate between 2D and 3D cases [3]. We measured the coalescence which is on a time scale of milliseconds depending on the radii of the involved droplets.

[1] Clark N., et al., 2017. Adv. Space. Res. 60 737
[2] Eremin, A., Baumgarten, S., Harth, K., Stannarius, R., 2011. Pys. Rev. Lett. 107, 268301.
[3] Hopper R., 1984, J. Am. Ceram. Soc. 67, C-262

CPP 47.7   Wed 16:45   H3
Re-entrant) Splashing of drops impacting on a heated plate at reduced pressure — •Kirsten Harth, Michiel van Limbeek, Paul Hoefnagels, and Detlef Lohse — Physics of Fluids, Max Planck Center and Universiteit Twente, Enschede, The Netherlands

Splashing drops capture our minds with their fascinating beauty - and splash control is highly relevant in a wide range of applications involving impacting drops. It is thus not surprising that diverse criteria for the splash threshold have been put forward over the last decades, with a recent breakthrough by Riboux and Gordillo (e.g. PRL 113 189901

(2014)). The effect of the surrounding gas is included via the mean free path, thus the theory also captures the disappearance of upon decrease of the ambient pressure. In our present understanding, identical drops remain intact at low impact velocities, while they always splash above a critical velocity.

Drop impact on heated surfaces in reduced pressure, however, bears a counterintuitive surprise: At temperatures below the static Leidenfrost point TL, the transition from deposition to splash is followed by another disappearance of splashing, before it reappears at larger impact velocity in a wide range of parameters. Above TL, splashing occurs at tremendously reduced impact velocity. We analyse this peculiar behaviour using different high speed imaging techniques.

CPP 47.8   Wed 17:00   H3
Morphology of liquid-liquid dewetting — •Roghayeh Shiri[1], Ralf Seemann[1], Dirk Peschka[2], and Barbara Wagner[2] — [1]University of Saarland, Saarbrucken, Germany — [2]Weierstrass Institute, Berlin, Germany.

We study the spinodal dewetting of nanometric thin liquid polystyrene (PS) films on liquid polymethyl-methacrylate (PMMA) substrates. The initial stage of dewetting consists of the amplification of thermal fluctuations driven by dispersion forces, eventually leading to the formation of holes with a preferred distance λ. According to theoretical predictions, the PS/air and the PS/PMMA interfaces shall evolve in a coupled way. As the surface tension of the PS/PMMA interface is way smaller than the surface tension of the PS/air interface, the amplitude of the corrugation of the PS/PMMA interface will be much larger than that of the PS/air interface. To determine the morphological evolution of the preferred wavelength λ and of the preferred holes distance, we follow the evolution of PS/air interface in situ by atomic force microscopy (AFM). The evolution of the PS/PMMA interface is explored ex situ by AFM using a lift up technique. By matching the PS/air and the PS/PMMA interfaces we can decide if the coupled corrugations of both interfaces evolve in phase or anti phase. We also explore the dependence of the preferred wavelength as function of PS film thickness and compare the result with theoretical predictions.

15 min. break

CPP 47.9   Wed 17:30   H3
Multiparticle Collision Dynamics Modeling of Nematic Liquid Crystal with Variable Order Parameter — •Shubhadeep Mandal[1] and Marco G. Mazza[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Loughborough University, Loughborough, United Kingdom

We have generalized the particle-based multiparticle collision dynamics (MPCD) method to model the hydrodynamics of nematic liquid crystals. Following Qian-Sheng theory [Phys. Rev. E 58, 7475 (1998)] of nematic liquid crystals, the spatial and temporal variations of the nematic director field and the nematic degree of order are described by a tensor order parameter. The principle idea is to assign a tensor quantity to each MPCD particle, whose average resembles the macroscopic tensor order parameter. The applicability of this new method is verified by performing several physical and numerical tests. We have tested: (a) the isotropic-nematic phase transition, (b) the annihilation dynamics of a pair of point defects, (c) the flow alignment of the nematic director in shear and Poiseuille flows, and (d) the velocity profile in shear and Poiseuille flows. We have found excellent agreement with existing literature. Additionally, we study the decay of force-dipole flow field in nematic liquid crystals. The present method can have far-reaching implications not only in modeling of nematic flows, but also to study the motion of colloids and microswimmers immersed in an anisotropic medium.

CPP 47.10   Wed 17:45   H3
Kinetic Monte Carlo simulations of thin film growth for pure and mixed films — •Eelco Empting, Miriam Klopotek, and Martin Oettel — Institut für angewandte Physik, Tübingen, Germany

We consider a binary lattice model for growth of demixing thin films, i.e. where two species of particles are deposited onto a substrate and undergo diffusion at and above it. Particle interactions include hardcore repulsion and nearest-neighbor attraction, the strength of which depends on the species of the particles involved. In KMC simulations of this model, we consider quite generally all sorts of single particle moves to neighboring sites, thus allowing for species-dependent diffu-

sion constants, desorption, and formation of cavities.

We studied the influence of the various parameters, most notably diffusion rates and interaction strengths, on the structure and evolution of a growing film. Among other things, this system was used to compare simulations to real-world growth experiments of a C60-CuPC blend film where we can identify the defining parameters leading to characteristic structure in the films.

CPP 47.11   Wed 18:00   H3
Classical density functional theory for ferrogels with distinguishable particles — •Segun Goh, Andreas M. Menzel, and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany

Classical density functional theory has been widely studied for liquidlike states of materials which consist of indistinguishable particles interacting via pairwise potentials. Meanwhile, there are materials, among which ferrogels provide one of the important examples, where the particles are fixed in an elastic polymer matrix. As particle neighbors do not change over time due to the fixation, particles are distinguishable by positions in those systems. In this talk, we discuss a density functional approach for such systems with distinguishable particles, considering a two-dimensional bead-spring lattice with magnetic dipoles at every bead as a model for ferrogels. We first introduce a mapping of the harmonic springs representing the elastic matrix onto a pairwise pseudo-interaction between indistinguishable particles. The mapping is justified by Monte-Carlo simulations of both the beadspring model and the frozen states of corresponding pseudo-interaction systems in combination with the density functional theory. We then formulate density functional theory for the dipole-spring model and investigate magnetostriction and compression moduli of ferrogels under magnetic interactions. We expect that our density functional approach may provide a route towards an understanding of a broad range of materials with particle inclusions.

CPP 47.12   Wed 18:15   H3
Crystallization of spheres with static and dynamic size dispersity — •Praveen Kumar Bommineni, Nydia Roxana Varela Rosales, Marco Klement, and Michael Engel — Institute for Multiscale Simulation, Friedrich-Alexander University Erlangen-Nürnberg, Nägelsbachstrasse 49b, 91052 Erlangen, Germany

Colloids are rarely uniform but follow a distribution of sizes, shapes, and charges. This dispersity can be inherent (static) or develop and change over time (dynamic). Despite a long history of research, the conditions under which non-uniform particles crystallize and which crystal forms is still not well understood. Here, we demonstrate that hard spheres with Gaussian radius distribution and dispersity up to 19% always crystallize if compressed slow enough, and they do so in surprisingly complex ways [1]. This result is obtained by accelerating event-driven simulations with particle swap moves for static dispersity and particle resize moves for dynamic dispersity. Above 6% dispersity, AB_2 Laves, AB_{13}, and a region of complex Frank-Kasper phases are found. The Frank-Kasper region includes a quasicrystal approximant with Pearson symbol oS276. Our findings are relevant for ordering phenomena in soft matter and alloys.
[1] P.K. Bommineni et al., arXiv:1811.00061.

CPP 47.13   Wed 18:30   H3
Elastic turbulence at low Reynolds numbers and its control — •Reinier van Buel, Christian Schaaf, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The properties of viscoelastic solutions are exceptionally applicable on the micron scale. For example, in microfluidic devices mixing and heat transfer are strongly enhanced. This is due to elastic turbulence [1], which bears similar qualities as inertial turbulence. The relevant dimensionless number characterizing viscoelastic fluids is the Weissenberg number, which compares the polymer relaxation time to the characteristic time of the flow dynamics.

Numerical solutions of the Oldroyd-B model in a two-dimensional Taylor-Couette geometry display a supercritical transition from the laminar Taylor-Couette to the occurence of a secondary flow [2]. The secondary flow is turbulent and caused by an elastic instability beyond a critical Weissenberg number. The order parameter, the time average of the secondary-flow strength, follows the scaling law $\Phi \propto (\mathrm{Wi} - \mathrm{Wi}_c)^\gamma$ with $\mathrm{Wi}_c = 10$ and $\gamma = 0.45$ and the power spectrum of the velocity fluctuations shows a power-law decay with a characteristic exponent.

Finally, we present first results on controlling the elastic instability through an oscillating rotation of the outer cylinder of the Taylor-Couette cell, with a frequency close to the characteristic relaxation time of the dissolved polymers.

[1] A. Groisman and V. Steinberg, Nature **405**, 53 (2000).
[2] R. Buel, C. Schaaf, H. Stark, Europhys. Lett. **124**, 14001 (2018).

CPP 47.14   Wed 18:45   H3

Gold nanoclusters at room temperature: are they soft matter? — •Luca M. Ghiringhelli, Bryan Goldsmith, Diego Guedes-Sobrinho, Jacob Florian, Jin-Xun Liu, Weiqi Wang, Juarez Da Silva, Ian Hamilton, and Matthias Scheffler — Fritz-Haber- Institut der Max-Planck-Gesellschaft, Berlin, Germany

Soft matter encompasses systems for which the predominant physical behaviors occur at an energy scale comparable with room-temperature (T=300 K) thermal energy. Here, we present a study of free-energy landscapes of neutral gold nanoclusters in the size ranges 10–13 (arXiv:1811.08062) and 25–40 (arXiv:1811.04438) atoms. Gold nanoclusters are interesting for their possible applications in gas sensing, pollution reduction, and catalysis. Our studies are based on extensive Born-Oppenheimer density-functional-theory replica-exchange molecular-dynamics sampling over a wide range of temperatures. We find that the long-standing question "At which *size* (neutral) gold clusters start favoring 3D vs 2D structures?" should be recast, at least in the size range between 10 and 13 atoms, into the question (here answered): "At which *temperatures* are 3D structures favored?". At T=300 K, we find that the typical activation barrier of Au–Au bonds is indeed comparable with the thermal energy, resulting in a continuous reshuffling of bonds and, in the size range 25–40 atoms, in low free-energy structures that significantly differ from the T=0 K structures. In these examples, gold nanoclusters seem indeed to match the definition of soft matter. This might have important implications for the characterization of the chemical reactivity of these systems.

CPP 47.15   Wed 19:00   H3

MIEZE spectroscopy of sub-picosecond collective dynamics in bulk liquid water — Olaf Soltwedel[1,2], •Leonie Spitz[3], Johanna K Jochum[3,4], Andreas Wendl[1], Christian Pfleiderer[1], and Christian Franz[3] — [1]Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — [2]Technische Universität Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany — [3]Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [4]Bayerisches Geoinstitut, Universität Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany

The anomalously large dielectric constant of water is intimately connected with a Debye relaxation peak in low frequency dielectric spectra. Despite intense research, a link between the molecular dynamics and the Debye relaxation peak, are still under heavy debate. Proposed mechanisms include translational and/or rotational motions, movement of free water molecules, collective relaxation of a cluster or hopping of defects in the hydrogen bond network. We used MIEZE (Modulation IntEnsity with Zero Effort) neutron spin echo spectroscopy, a high resolution time of flight technique, to measure the dynamic structure factor ($S(q,t)$) of water over an exceptional dynamical range (0.01 up to 1000ps). Consistent with the literature, we find the bulk transverse diffusion on length scales from 0.1/Å up to 0.4/Å. As our main result, reveals at least two more processes on sub-picosecond time-scales. This provides direct evidence of a vibration and/or delocalization of hydrogen larger than the intermolecular distance as proposed [1].

[1] A. Arbe et al. PRL 117, 185501 (2016)