DY 18: Soft matter

Time: Wednesday 14:00–16:30

Location: MA 001

Invited Talk　　　　　　　DY 18.1　Wed 14:00　MA 001
Rate Dependence and Role of Disorder in Linearly Sheared Two-Dimensional Foams. — •Martin Van Hecke, Gijs Katgert, and Matthias Moebius — Kamerlingh Onnes Lab, PObox 9504 2300 RA Leiden, the Netherlands

We experimentally probe the rheology of two dimensional foams sandwiched between the fluid phase and a top-plate, and find that these flows depend crucially on both the applied strain rate and the degree of disorder of the foam: (1) Disordered, bidisperse foams exhibit rate dependent flow profiles, which become increasingly shear-banded for large shear rates. (2) Ordered, monodisperse foams exhibit rate independent flows.

These findings are captured in a model in which the averaged drag forces between bubble and top plate are balanced by the inter-bubble drag forces. We show that nonlinear scaling of these forces and rate dependent flows are intimately connected.

The fact that disorder plays such a crucial role for the foam flow, evidences that the translation from individual inter-bubble drag forces to the average inter-bubble drag forces is nontrivial. We find that for disordered foams the average inter-bubble drag forces scale differently from the individual inter-bubble drag forces. This is consistent with earlier suggestions that the averaged viscous drags are enhanced over what might be expected from the local interactions, due to disordered, non-affine, bubble motion. We discuss how anomalous scaling of bulk properties caused by non-affine motion at the micro scale appears to be a general feature of disordered systems close to jamming.

DY 18.2　Wed 14:30　MA 001
Mesoscale, particle-based simulations of binary mixtures and microemulsions — •Thomas Ihle and Daniel Kroll — Department of Physics, North Dakota State University, Fargo, ND, 58105, USA

An appealing algorithm for complex fluids introduced by Malevanets and Kapral, often called Stochastic Rotation Dynamics (SRD), describes a fluid by means of particles which undergo efficient multiparticle collisions. The algorithm has been successfully applied to study the behavior of polymers, colloids and vesicles.

Here, we use a recent generalization of this algorithm for binary mixtures [1,2]. We present results for the demixing of a mixture such as the phase diagram, interface fluctuations and the surface tension of a droplet. We show how Ginzburg-Landau free energy functionals including gradient terms can be derived from the microscopic collision rules. Expressions for the equation of state and the phase diagram are shown to be in excellent agreement with numerical results.

To describe microemulsions, a third phase of surfactant molecules is introduced which consists of rigid objects. We show how objects of arbitrary shape can be efficiently embedded in the SRD-fluid. The phase diagram and results for emulsification will be presented.
[1] T. Ihle, E. Tuzel, D.M. Kroll, Europhys. Lett. 73 (2006) 664.
[2] E. Tuzel, G. Pan, T. Ihle and D. M. Kroll, Europhys. Lett. 80 (2007) 40010.

DY 18.3　Wed 14:45　MA 001
Effective Interactions in Like-Charged Colloidal Mixtures and Cluster Formation — •A. V. Anil Kumar[1] and Juergen Horbach[2] — [1]Institut für Physik, Universität Mainz, Staudinger Weg 7, 55099 Mainz — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln

We consider binary mixtures of like-charged colloidal particles of large size disparity. Using molecular dynamics simulations, the depletion interaction between the big colloidal particles mediated by a fluid of small particles is calulated. Attention is given to the region in parameter space where there is an effective attractive interaction between the large spheres. Our results indicate that indeed there exists an attractive force between two large spheres when the interaction between the large and small spheres are non-additive and highly repulsive. This attractive interaction is due to the overlap of depletion regions around two big spheres formed due to the high repulsion between large and small spheres. The strength of this effective attraction depends on the strength of large-small repulsion and also on the number ratio between the large and small particles. In this attractive region, we simulated a bulk system, where we observed cluster formation among the big

particles. The cluster size distribution decays exponentially with cluster size, which is in agreement with experimental observations. At higher volume fractions, the cluster size distribution develops a two peak structure. This may be seen as a precursor to phase separation. The detailed results of molecular dynamics simulations and their connection with experimental observations will be discussed.

DY 18.4　Wed 15:00　MA 001
Dynamical Simulations Of Colloids In Optical Tweezers — •Rudolf Weeber and Jens Harting — Institute For Computational Physics, University Of Stuttgart, Pfaffenwaldring 27, D-70569 Stuttgart

Dynamical Simulations Of Colloids In Optical Tweezers Optical tweezers are important tools in the study of colloidal suspensions outside of equilibrium, because they make it possible to perturb the system in a controlled manner. We present simulations of a colloid dragged through both, a colloidal crystal and a polymer suspension using an optical tweezer modeled as a moving parabolic potential. From the behavior of the dragged particle within the trap and the surrounding crystal, dynamical properties like drag forces and the rearrangement of surrounding particles in the suspension are obtained. The simulations for both systems are compared to experiments. For the polymer suspension, we find a linear velocity-force relation. At high polymer concentrations, we find a significant accumulation of polymers in front of the dragged colloid. This leads to an increased drag force, that cannot be explained by the Stokes-Einstein-Relation. For the colloidal crystal, the drag force is non-linear with respect to velocity. Also, the details of the inter-colloid potential play an important role in the velocity-force relation. We also compare two simulation techniques - namely Brownian Dynamics and Stochastic Rotation Dynamics - to evaluate the impact of complex hydrodynamic interactions on these experiments.

DY 18.5　Wed 15:15　MA 001
From soliton staircases to strain density waves: Monte Carlo simulations of surface-induced deformation of soft colloidal crystals — David Yu-Hang Chui[1], •Surijit Sengupta[2], and Kurt Binder[1] — [1]Institut für Physik, Johannes-Gutenberg-Universitüt, Staudingerweg 7, 55099 Mainz, Germany — [2]S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700098, India

Two dimensional colloidal crystal interacting with an inverse power law potential was studied using Monte Carlo simulations. Two structured walls, which are created by choosing two rows of particles fixed in the positions of the triangular lattice, provide the confinement to the system. By varying the distance between two walls, the deformation of the two dimensional colloid is induced and typical soliton staircase can be observed. The strain in the system was also calculated and the strain density wave superstructure was found in the different thicknesses of the strips.

DY 18.6　Wed 15:30　MA 001
Ground-state properties of thick flexible polymers — •Thomas Vogel[1], Thomas Neuhaus[2], Michael Bachmann[1], and Wolfhard Janke[1] — [1]Institute for Theoretical Physics, University of Leipzig, PF 100 920, 04009 Leipzig — [2]John von Neumann Institute for Computing, Forschungszentrum Jülich, 52425 Jülich

We investigate ground-state properties of a simple model for flexible polymers, where the steric influence of monomeric side-chains is effectively introduced by a thickness constraint [1]. Thickness is defined via the global radius of curvature [2]. From parallel tempering and flat-histogram computer simulations, we find a strong thickness dependence of the conformational topology of the ground-state structures. A systematic analysis for short polymers allows for a thickness-dependent classification of the dominant ground-state topologies. It turns out that helical structures, strands, rings, and coils are natural, intrinsic geometries of such linelike objects.
[1] T. Neuhaus, O. Zimmermann, and U.H.E. Hansmann, Phys. Rev. E 75, 051803 (2007).
[2] O. Gonzalez and J. Maddocks, Proc. Natl. Acad. Sci. USA 96, 4769 (1999).

DY 18.7   Wed 15:45   MA 001

Conformational transitions of flexible polymers — •Stefan Schnabel, Michael Bachmann, and Wolfhard Janke — Institut für Theoretische Physik Universität Leipzig

We investigate collapse and crystallization of flexible homopolymers by means of multicanonical computer simulations of a simple off-lattice bead-spring polymer model with FENE (finitely extensible nonlinear elastic) bond potential [1] and intramonomeric Lennard–Jones interaction.

Beside the well known Theta transition we also observe another transition at lower temperatures which is expected to be the liquid-solid transition. This is indicated by sharp energetic fluctuations as signalized by the specific heat. The crystallized polymer structures possess similarities to ground states of pure Lennard-Jones clusters. From our results, we also conclude that crystallization and collapse transition remain well separated in the thermodynamic limit [2].

[1] R. B. Bird, C. F. Curtiss, R. C. Armstrong and O. Hassager, Dynamics of Polymeric Liquids, 2nd ed., 2 vols. (Wiley, New York, 1987). [2] D. F. Parsons and D. R. M. Williams, J. Chem. Phys 124, 221103 (2006)

DY 18.8   Wed 16:00   MA 001

Steric molecular recognition: Selecting Components of Hard Rod Mixtures — •Thomas Gruhn and Andreas Richter — Max Planck Institute for Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany

The mechanisms of molecular recognition are of great relevance for the development of specific pharmaceutical agents. One important selection method is based on the geometrical matching of the receptor and the molecule of interest. A large molecule cannot enter a small cavity, but, at first sight, a molecule cannot be too small to enter a large cavity. However, we have found that suitably shaped cavities in a substrate can select molecules of a specific size from a polydisperse system by purely steric interactions. We have performed Monte Carlo simulations of a system of hard rods with a length polydispersity in contact with a hard substrate. The planar substrate has rectangular cavities, that match geometrically to one rod component of the mixture. The simulations show that the corresponding rod component can be successfully selected from the system of rods. A direct usage of this effect is the preparation of colloidal rod systems with a narrow length distribution.

DY 18.9   Wed 16:15   MA 001

Adaptive molecular resolution via a continuous change of the phase-space dimensionality: Theory and Application — •Luigi Delle Site, Matej Praprotnik, and Kurt Kremer — Max-Planck Institute for Polymer Research, Mainz

For the study of complex synthetic and biological molecular systems by computer simulations one is still restricted to simple model systems or to by far too small time scales. To overcome this problem multiscale techniques are being developed. However in almost all cases, the regions treated at different level of resolution are kept fixed and do not allow for a free exchange. We here present a robust computational method and a basic theoretical framework for an efficient and flexible coupling of the different regimes. The approach leads to the concept of "geometry induced phase transition" and to a counterpart of the equipartition theorem for fractional degrees of freedom. The efficiency of the presented approach is illustrated by the application to several systems.