CPP 34: Colloids and Complex Liquids II

Time: Thursday 15:00–18:45 Location: C 130

Invited Talk CPP 34.1 Thu 15:00 C 130

Colloidal quasicrystals: from their discovery to photonic applications — •Stephan Förster[1], Alexander Exner[1], Sabine Rosenfeldt[1], Jan Perlich[2], and Peter Lindner[3] — [1]Physikalische Chemie I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]HASYLAB/DESY, 22607 Hamburg, Germany — [3]Institut Laue Langevin, 38042 Grenoble, France

Micelles are the simplest example of self-assembly found in nature. As many other colloids, they can self-assemble in aqueous solution to form ordered periodic structures. These structures so far all exhibited classical crystallographic symmetries. Using small-angle neutron and x-ray diffraction, for the first time quasi-crystalline micellar phases were observed exhibiting 12-fold and 18-fold diffraction symmetry. Colloidal water-based quasicrystals are physically and chemically very simple systems. This discovery is of particular importance, as it opens a new versatile route to quasicrystalline photonic band gap materials via water-based colloidal self-assembly techniques.

CPP 34.2 Thu 15:30 C 130

Regular packings on periodic lattices — •Tadeus Ras[1,3], Rolf Schilling[1], and Martin Weigel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [2]Applied Mathematics Research Centre, Coventry University, England — [3]Present address: Fachbereich Physik, Universität Konstanz, Germany

We investigate the problem of packing identical hard objects on regular lattices in d dimensions. Restricting configuration space to parallel alignment of the objects, we study the densest packing at a given aspect ratio X. For rectangles and ellipses on the square lattice as well as for biaxial ellipsoids on a simple cubic lattice, we calculate the maximum packing fraction $\varphi_d(X)$. It could be proved to be continuous with an infinite number of singular points $X_\nu^{\min}$, $X_\nu^{\max}$ $\nu = 0, \pm1, \pm2, \ldots$. In two dimensions, all maxima have the same height, whereas there is a unique global maximum for the case of ellipsoids. The form of $\varphi_d(X)$ is discussed in the context of geometrical frustration effects, transitions in the contact numbers and number theoretical properties. Implications and generalizations for more general packing problems are outlined [1].

[1] T. Ras, R. Schilling and M. Weigel, Phys. Rev. Lett. **107**, 215503 (2011)

CPP 34.3 Thu 15:45 C 130

Fluid-mediated gelation of hard spheres — •Andrea Fortini — Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, Universitätsstraße 30, D-95440 Bayreuth, Germany

We propose a minimal model for the description of the fluid-mediated gelation of purely repulsive colloidal particles described in recent experimental work [Koos, E. and Willenbacher, N. (2011). Science, 331, p.897]. We find that the addition of non-wetting fluid droplets to a suspension of pure hard spheres can lead to the formation of clusters that can eventually percolate and form a gel. We show with Brownian dynamics computer simulations of a binary mixture of colloids and droplets that gelation is due to a percolation transition compatible with diffusion limited cluster aggregation and that the dynamical and mechanical properties are those of a gel of colloidal particles.

CPP 34.4 Thu 16:00 C 130

Hard sphere crystals and crystal-liquid interfaces — •Martin Oettel — Mainz University, Institute of Physics

Density functional theory in the form of Fundamental Measure Theory (FMT) is capable of describing hard sphere crystals and interfaces very accurately. With FMT as a benchmark, we discuss the merits and shortcomings of simpler and more popular models (Ramakrishnan-Youssouff and Phase Field Crystal model). Furthermore we address the concept of crystallinity modes and the associated order parameter profiles at crystal-liquid interfaces as these are central ingredients for coarse-grained phase-field modelling employed in materials science.

CPP 34.5 Thu 16:15 C 130

Fixing contact angles in model colloid-polymer mixtures — •Antonia Statt, Alexander Winkler, Peter Virnau, and Kurt Binder — Institute of Physics, JGU Mainz , 55128 Mainz

We study a continuous version of the Asakura-Oosawa model with grandcanonical simulations as a model system for colloid-polymer mixtures. By applying a novel computational scheme with a "mixed Hamiltonian" the system is slowly driven from bulk to planar confinement and vice versa, and we are able to determine interfacial free energies with respect to walls and contact angles. By varying the colloid-wall interaction range while leaving the polymer-wall interaction constant, we are able to fix arbitrary contact angles ranging from complete wetting of colloids to complete wetting of polymers at the wall. These investigations may not only guide future experiments but also form the basis for the study of heterogeneous nucleation in complex geometries such as cylindrical and spherical confinement.

CPP 34.6 Thu 16:30 C 130

Two-dimensional percolated networks induced by an uniform external field. — •Heiko Schmidle[1], Carol K. Hall[2], Orlin D. Velev[2], and Sabine H. L. Klapp[1] — [1]Technische Universität Berlin — [2]North Carolina State University

In this work we present results of a theoretical investigation of induced dipoles mixed with particles that contain two induced dipoles, one pointing into the field and the other one opposite to it. Our model is based on current experimental works where such particles are synthesized and interesting self-assembly is observed [1]. Induced dipoles tend to form chains into the external field direction [2]. Particles that contain two dipole moments are similar to quadrupolar particles and are able to build structures perpendicular to the external field. The mixture allows the assembly into two-dimensional networks induced by an one-dimensional field and this effect is of great interest in synthesizing new responsive materials. The formation of dipoles without field was also studied recently [3]. We use Monte-Carlo simulations to study the assembly of such particles and the physical properties of the resulting networks. Further we focus on the influence of macroscopic parameters like concentration and density on these properties.

[1] S. Gangwal, A. Pawar, I. Kretzschmar, and O. D. Velev, Soft Matter 6, 1413 (2010).

[2] H. Schmidle and S. H. L. Klapp, J. Chem. Phys. 134, 114903 (2011).

[3] H. Schmidle, C. K. Hall, O. D. Velev, and S. H. L. Klapp, Soft Matter (2011), accepted.

15 min break

CPP 34.7 Thu 17:00 C 130

Predicting DNA-mediated colloidal interactions with a simple self-consistent mean-field model — •Stefano Angioletti-Uberti, Bortolo Mognetti, Patrick Varilly, and Daan Frenkel — Department of Chemistry, University of Cambridge, Lensfield Road, CB2 1EW Cambridge, UK

We present a general model able to describe with semi-quantitative accuracy the interaction energy between micron-sized DNA coated colloids (DNACCs). The generality of this theory, based on a self-consistent mean-field approach, allows to treat under the same unifying framework arbitrary mixtures of DNACCs functionalized with various types of DNA-based constructs and nucleotides sequences. We compare our theory with full numerical results from Monte Carlo simulations and we discuss in-depth the thermodynamic consistency of our approach, paying attention to highlight the assumptions in our model and possible ways to relax them. It is expected that the present theory will provide a usefull tool for fast, off-the-shelf calculations of DNA-coated colloids interactions.

CPP 34.8 Thu 17:15 C 130

Modeling swimming active droplets — •Maximilian Schmitt and Holger Stark — Institut für Theoretische Physik, TU Berlin

In a recent attempt to build an active microswimmer, a micron-sized droplet of bromine water was placed into a surfactant laden oil medium such that the surfactant molecules spontaneously assemble at the droplet interface [1]. Experiments revealed that due to a bromination reaction of the surfactant (mono-olein), the surface tension locally increases. At the same time these surfactants with a higher surface tension are readily replaced by surfactants from the surrounding oil phase. As a result, a steady gradient of surface tension on the droplet is created. Since an interface with higher surface tension pulls more strongly

on a surrounding liquid than one with a lower surface tension, the surface tension gradient on the droplet generates the so-called Marangoni flow.

In order to understand the swimming mechanism, we establish a model based on a free energy functional for the droplet interface. The free energy accounts for the mixing entropy, interactions between the surfactant molecules, and adsorbtion/desorbtion of surfactants from/into the bulk medium. After also taking into account the bromination and the Maranogi flow, we arrive at a reaction-advection diffusion equation on a sphere. Numerical simulations are carried out in order to obtain the flow field at the interface and the swimming trajectory of the droplet.

[1] Shashi Thutupalli *et al* 2011 *New J. Phys.* **13** 073021

CPP 34.9 Thu 17:30 C 130

Self-assembled nematic defect-structures for Janus beads — •Michael Melle[1], Sergej Schlotthauer[1], and Martin Schoen[1,2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [2]Department of Chemical and Biomolecular Engineering, North Carolina State University, 911 Partners Way, Raleigh, NC 27695, U.S.A.

We present Monte Carlo simulations of a colloid embedded in a nematic liquid crystal host. Employing different alignment scenarios for the liquid crystal molecules on the surface of the colloid our model is able to reproduce known defect structures of the liquid crystal, such as Saturn ring, surface ring, or Boojum defect to high accuracy and over a wide range of parameters like temperature, pressure or strength of alignment. However, the main focus of this study is on inhomogeneous, spherical colloids such as Janus beads. Despite the large interest that Janus beads have attracted in the last decade, almost no work has been done on the defect structures generated by them. Therefore, we also develop different alignments for different sides of the colloid. We are able to reproduce experimentally known defect structures for Janus beads. In addition, we also predict new topologies. Furthermore, we see transitions between different defect structures induced by a slight decrease of temperature, which is a novel observation as well.

CPP 34.10 Thu 17:45 C 130

Particles as emulsion stabilizers: a simulation study — •Jens Harting[1,2], Stefan Frijters[1], and Florian Günther[1] — [1]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands — [2]Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

Emulsions stabilized by particles are ubiquitous in the food and cosmetics industry, but our understanding of the influence of microscopic fluid-particle and particle-particle interactions on the macroscopic rheology is still limited. Modern simulation algorithms based on a multicomponent lattice Boltzmann model to describe the solvents combined with a molecular dynamics solver for the description of the suspended particles allow to tune the particle size, shape, wettability and surface tensions between the fluids. Further, they are ideal candidates to harness the power of today's largest available supercomputers allowing to model small macroscopic systems with microscopic resolution.

We report on the adsorption of spherical or ellipsoidal particles to liquid interfaces and demonstrate the existence of stable and semi-stable equilibrium states. On larger scales, different phases of stabilized emulsions have been found. While Pickering emulsions are already known for more than a century, so-called bicontinuous interfacially jammed emulsion gels (Bijels) where only predicted recently. The particles can fully arrest domain growth and a transition between both phases can be found by tuning the concentration, contact angle, or fluid ratio. Further, by tuning the particle shape additional geometrical degrees of freedom add additional time scales to the arrest of domain growth.

CPP 34.11 Thu 18:00 C 130

Resonances arising from hydrodynamic memory - The Color of Brownian motion — •Sylvia Jeney[1], Matthias Grimm[1], Flavio Mor[1], Laszlo Forro[1], and Thomas Franosch[2] — [1]Laboratory of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [2]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Germany

Observation of the Brownian motion of a small probe interacting with its environment is one of the main strategies to characterize soft matter. Initially, the particle is driven by rapid collisions with the surrounding solvent molecules, referred to as thermal noise. Later, the friction between the particle and the viscous solvent damps its motion. Conventionally, thermal force is taken to be characterized by a Gaussian white noise spectrum. The friction is assumed to be given by the Stokes drag, suggesting that motion is overdamped at long times, when inertia becomes negligible. Here, we measured the noise spectrum of the thermal forces by tracking with high resolution a single micron-sized sphere suspended in a fluid, and confined by a stiff optical trap [1]. Coupling between sphere and fluid gives rise to hydrodynamic memory [2] and a resonance, equivalent to a colored peak in the power spectral density of the sphere*s thermal fluctuations. Our results reveal that motion is not overdamped, even at long times. In view to exploit the particle-fluid-trap system as a nanomechanical resonator, we disentangle the two regimes in which the detected resonance is either sensitive to the fluid properties or to the particles mass. [1] Jeney et al. Nature 2011. [2] Jeney et al. PRL 2008.

CPP 34.12 Thu 18:15 C 130

Magnetic nanorods: A Monte Carlo study — •Carlos E. Alvarez and Sabine H. L. Klapp — Institut für Theoretische Physik, TechnischeUniversität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We perform Monte Carlo simulations of model stiff magnetic nanorods composed of several magnetic hard spheres. We study the thermodynamic properties as well as the structure formation and percolation properties of the system with and without an applied external magnetic field for various densities and temperatures. We measure a critical path approximation for the conductance of the system [1] and observe how it is affected by the length of the rods, the temperature of the system and the presence and strength of an applied external field. We also look at dipolar prolate spheroids [2] as models for magnetic nanorods and compare the results with the multi-sphere rod model.

[1] G. Ambrosetti, C. Grimaldi, I. Balberg, T. Maeder, A. Danani and P. Ryser, *Phys. Rev. B*, **81**, 155434 (2010).

[2] G. J. Zarragoicoechea, J.-J Weis and D. Levesque, *Mol. Phys.*, **74**, 629 (1991).

CPP 34.13 Thu 18:30 C 130

Magnetic particles with shape anisotropy — Sofia Kantorovich[1,2] and •Elena Pyanzina[2] — [1]Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart, Germany — [2]Ural Federal University, Lenin av 51, 620083, Ekaterinburg, Russia

Anisotropic particles form the cutting edge of dipolar soft matter research as they correspond completely to the idea of fine tuning and designing new materials with controllable properties. In this contribution we present a theoretical study and computer simulations on the ground states, and room temperature behaviour of magnetically capped colloids, magnetic ellipsoids, cylinders and cubes. We analyse in detail how the particle anisotropy can be used in fine-tuning of the properties and macro responses of the systems.