DY 5: Soft matter

Time: Monday 14:45–16:45 Location: ZEU 255

DY 5.1 Mon 14:45 ZEU 255

Thickness-Dependent Secondary Structure Formation of Tubelike Polymers — •Thomas Vogel[1], Thomas Neuhaus[2], Michael Bachmann[1], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, D-04009 Leipzig, Germany — [2]John von Neumann Institute for Computing (NIC), Forschungszentrum Jülich, D-52425 Jülich, Germany

By means of sophisticated Monte Carlo methods, we investigate the conformational phase diagram of a simple model for flexible polymers with explicit thickness [1,2]. The thickness constraint, which is introduced geometrically via the global radius of curvature of a polymer conformation, accounts for the excluded volume of the polymer and induces cooperative effects supporting the formation of secondary structures [3]. In our detailed analysis of the temperature and thickness dependence of the conformational behavior for classes of short tubelike polymers, we find that known secondary-structure segments like helices and turns, but also ringlike conformations and stiff rods are dominant intrinsic topologies governing the phase behavior of such cooperative tubelike objects. This shows that the thickness constraint is indeed a fundamental physical parameter that allows for a classification of generic polymer classes.

[1] T. Vogel, T. Neuhaus, M. Bachmann, W.Janke, Europhys. Lett. (2009) (in print)
[2] T. Vogel, T. Neuhaus, M. Bachmann, W.Janke, to be published
[3] J.R. Banavar, A. Maritan, Rev. Mod. Phys. **75**, 23 (2003)

DY 5.2 Mon 15:00 ZEU 255

Self-assembling network and bundle structures in systems of rods and crosslinkers — Raghunath Chelakkot[1], Reinhard Lipowsky[2], and •Thomas Gruhn[3] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52428 Jülich — [2]MPI for Colloids and Interfaces, Science Park Golm, D-14424 Potsdam — [3]Johannes Gutenberg Universität Mainz, Inst. f. Anorg. u. Analyt. Chemie, D-55099 Mainz

Self-assembling structures are studied in a binary system of long and short spherocylinders. The short spherocylinders have an adhesive site on both ends with which they can bind to the long spherocylinders. In this way, they act as crosslinkers that may interconnect a pair of long rods. In a similar way, network structures are formed by crosslinked actin filaments in the cytoskeleton of living cells. With the help of Monte Carlo simulations, the structure of crosslinker-mediated rod assemblies has been studied systematically and the critical behavior at the percolation threshold has been studied. The system shows a complex phase behaviour, including the formation of bundles of parallel rods and a transition to a three-dimensional, low-densitiy network. Bundles occur both in percolated and non-percolated systems. The same observations have been made for crosslinked actin filament networks in living cell. In a certain range of rod and crosslinker concentrations, the amount of bundling rods is a non-monotonic function of the adhesive strength.

DY 5.3 Mon 15:15 ZEU 255

Phase behaviour and demixing of a two dimensional oligomer-solvent system — •Daniel Reith, Peter Virnau, Katarzyna Bucior, Leonid Yelash, and Kurt Binder — Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz

We present the complete phase diagram of a two dimensional off-lattice oligomer-solvent mixture which describes the behaviour of hexadecane in supercritical CO2 in a slit pore geometry. A detailed finite-size analysis of our grandcanonical Monte Carlo data shows that the system belongs to the two dimensional Ising universality class. Based on this analysis we study demixing by spinodal decomposition with Molecular Dynamics simulations.

DY 5.4 Mon 15:30 ZEU 255

Test particle limit for the pair structure of quenched-annealed fluid mixtures — •Matthias Schmidt — Theoretische Physik II, Universität Bayreuth, Universitätsstraße 30, D-95440 Bayreuth, Germany

A novel route to the pair structure of quenched-annealed fluid mixtures is presented. The bulk two-body partial pair correlation functions of the mixture are identified with the one-body density distributions in an external potential that models a test particle fixed at the origin. Quenched-annealed (or replica) density functional theory is used to calculate the inhomogeneous one-body density distributions. A closed theory is obtained by using an exact sum rule that equates two different expressions for the cross pair correlation function between unlike species. Results for binary quenched-annealed hard sphere mixtures demonstrate good agreement with computer simulation data, improving over results from the replica Ornstein-Zernike equations using the direct correlation functions, obtained as second functional derivatives of the quenched-annealed excess free energy functional, as input.

DY 5.5 Mon 15:45 ZEU 255

Phase behavior of a dipolar monolayer: An integral equation study — •Liang Luo[1,2] and Sabine H. L. Klapp[1] — [1]Institut für Theoretische Physik, Arnimallee 14, Freie Universität Berlin, D-14195 Berlin, Germany — [2]Institute of Theoretical Physics, Chinese Academy of Science, Beijing 100080, China

Using integral equation theory in the Reference Hypernetted Chain (RHNC) approximation we investigate the structure and phase behavior of a dipolar hard sphere (DHS) monolayer. The dipole orientations of the particles are confined to the plane, reflecting the strong tendency of three-dimensional dipoles to orient along in-plane directions. The phase behavior is studied with an instability analysis for a wide range of densities. In agreement with simulation results, we find that the cluster- and chain-formation dominates the low density region around the spinodal temperature. With the density increasing, we observe larger contact numbers, signalling longer average chain lengths and more complicated structures such as crossing chains. In the high density region, there is no obvious indication for ferroelectric long-range correlations, contrary to the behavior of three-dimensional dipolar fluids. The instability analysis rather indicates crystallization at these high densities.

DY 5.6 Mon 16:00 ZEU 255

A wedge-shaped polarizing analyzer for the TOF spectrometer FOCUS - Ray-trace MC simulations and experiments — •Ralf Ackermann[1,2], Uwe Filges[3], Michael Schneider[1], Jochen Stahn[1], Lothar Holitzner[3], Thierry Strässle[1], Jan Peter Embs[1,2], and Rolf Hempelmann[1] — [1]Saarland University, DE — [2]LNS, ETH Zurich and PSI, CH — [3]LDM, PSI, CH

For the cold neutron TOF spectrometer FOCUS at the Swiss Spallation Neutron Source, we are developing a polarization option, which can be used, e.g., for the separation of coherent and spin-incoherent scattering contributions. Our design is based on a wedge-shaped stack of horizontally bent polarizing magnetized supermirrors covering continously the entire scattering range of 120 deg. In our setup, we use remanent magnetized FeCoV/NiN supermirrors produced at PSI. The supermirrors are surrounded by a magnetic guide field of 4.5 mT at the center position. Using the neutron ray-trace Monte-Carlo simulations, we calculated polarization and transmission properties of a 4.8 deg section. We performed test measurements on an analyzer prototype consisting of a stack of 30 supermirrors covering about 2 deg. On a polarized incoming beam of 1 mm x 40 mm dimension and varying wavelength we measured polarization values up to 95% and transmission coefficients up to 75% (6 Å). To further optimize the performance of our setup, we performed finite element calculations of the magnetic guide field and checked these results with a measurement after modifying the guide around the analyzer's entry. Results of our simulations and measurements will be presented and discussed here.

DY 5.7 Mon 16:15 ZEU 255

Ordering of colloidal particles on quasicrystalline substrates with decagonal or tetradecagonal symmetry — •Michael Schmiedeberg and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10632 Berlin, Germany

Quasicrystals are non-periodic solids that nevertheless have a long-range positional order. They possess rotational point symmetries, such as five, eight, ten, or twelve-fold rotational axes that are not allowed in periodic crystals. However, not for all rotational symmetries stable quasicrystals exist in nature. For example, quasicrystals with seven-fold rotational axes have not been observed so far.

By using Monte-Carlo simulations, we study charged-stabilized col-

loidal particles in two-dimensional decagonal or tetradecagonal potentials, which in experiments are realized by five or seven interfering laser beams, respectively. For intermediate light intensities and special particle densities, orderings corresponding to Archimedean-like tilings occur in both potentials. A closer analysis of these structures reveals substantial differences between the decagonal and the tetradecagonal potential. For example, there are large areas with almost periodic ordering in the tetradecagonal but not in the decagonal potential. We give a possible explanation of this behavior by analyzing properties of the substrate potential that depend on whether its rotational symmetry is realized in nature or has never been observed.

DY 5.8 Mon 16:30 ZEU 255

Structure and high-frequency viscosity in dispersions of charge-stabilized colloidal spheres — •Marco Heinen and Gerhard Nägele — Institut für Festkörperforschung, Teilinstitut Weiche Materie, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

The short-time effective viscosity of suspensions of charge-stabilized colloidal spheres is calculated by means of a renormalized density fluctuation expansion. Systems at various volume fractions, particle charges and salt concentrations are considered.

The only input required for this calculation is the static structure factor which we obtain from appropriate Ornstein-Zernicke integral equation theories. In particular, we investigate a simple modification of the well-known rescaled mean spherical approximation (RMSA) suggested by Snook and Hayter, which includes a microionic background correction that tends to compensate the typical underestimation of microstructure by the RMSA. The background-corrected RMSA is in good agreement with our simulation data and the computationally more expensive Rogers-Young scheme.