DY 12: Soft Matter I

Time: Tuesday 14:30–16:00

DY 12.1　Tue 14:30　H47

^{2}H NMR study on the molecular motion of water in hydrated myoglobin — •Sorin Adrian Lusceac and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 6, 64289 Darmstadt

The physiological properties of proteins are strongly dependent on the water dynamics (WD) in their hydration shell. Hence, ^{2}H NMR spin-lattice relaxation and solid-echo experiments were performed to investigate the WD in a water/myoglobin mixture. The obtained rotational correlation times agree with those from dielectric spectroscopy measurements. They can be described by an Arrhenius law in the high temperature range, with the possibility of a weak crossover to a second Arrhenius dependence at about 220K. No evidence for a fragile-to-strong transition, as proposed in literature[1], is found, consistent with results for hydrated elastin and collagen[2, 3]. From the spectral analysis, we conclude that at high temperatures (>230K) the WD is isotropic while at lower temperatures (<220K) anisotropic large-angle dynamics is observed. We performed random-walk simulations for several anisotropic WD models and discuss the resulting spectra in connection with the experimental results.

[1] S.-H. Chen et al., Proc. Natl. Acad. Sci. 103 (2006) 9012.
[2] M. Vogel, Phys. Rev. Lett. 101 (2008) 225701.
[3] S. A. Lusceac et al., Biochim. Biophys. Acta 1804 (2010) 41.

DY 12.2　Tue 14:45　H47

Mechanical Properties of Bilayer Membrane and Inclusion — •Giovanni Marelli — Institut für theoretische Physik Friedrich-Hund-Platz 1 D-37077 Göttingen

The presence of a hydrophobic inclusion in a bilayer membrane modifies the shape and the mechanical properties of the membrane. Due to the surface tension between the inclusion and the hydrophobic monomers the region around the inclusion is enriched in chains and the membrane bends around the defect. After the enriched zone the membrane is deplected and is prone to the formation of a pore. In this talk is presented a coarse-grained solvent-free model to study polymersome/nanoparticle and lipid vesicle/peptide inclusions. In the first system, we investigate the condition of stability of the nanoparticle with and without the presence of defectants that decrease the surface tension of the inclusion. In the second one the attention is placed upon to the radial profile of the bending of the membrane around the peptide, which is compared to a continum elastic model, to the increase of the membrane tension and to the packing effect of the lipids around the peptide.

DY 12.3　Tue 15:00　H47

Phase behavior of colloidal suspensions in critical solvents — •Thomas Friedrich Mohry[1,2], Anna Maciołek[1,2,3], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, D-70569 Stuttgart, Germany — [2]Universität Stuttgart, Institut für Theoretische und Angewandte Physik, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [3]Institute of Physical Chemistry, Polish Academy of Sciences, Department III, Kasprzaka 44/52, PL-01-224 Warsaw, Poland

Colloidal systems are important both as model systems for statistical physics and for applications in material science. Close to a continuous phase transition of the solvent (e.g. the critical point of the mixing-demixing transition in a binary mixture) the correlated fluctuations result in an effective force between the immersed colloids, the so called critical Casimir forces. They exhibit the remarkable feature of universality and are sensitive to the temperature, the boundary conditions imposed by the colloids and the composition of the solvent. We present first theoretical results, concerning the influence of these critical Casimir forces on the phase behavior of the colloids.

DY 12.4　Tue 15:15　H47

Time-dependent primitive path analysis — •Jixuan Hou[1], Carsten Svaneborg[2], Gary Grest[3], and Ralf Everaers[1] — [1]École Normale Supérieure de Lyon — [2]University of Aarhus — [3]Sandia National Laboratories

The complex viscoelastic properties of polymer liquids are due to the presence of topological constraints on a molecular scale. On a microscopic scale chains can slide past each other, but their backbones cannot cross. The standard model of polymer dynamics, the tube model, assumes that entanglements confine chain fluctuations to a narrow tube-like region along a so-called *primtive path" which follows the coarse-grained chain contour.

Primitive paths were originally introduced in a thought experiment as the shortest paths into which chains with fixed endpoints can contract without crossing each other. A few years ago, we have shown how to perform a corresponding primitive path analysis (PPA) of computer generated conformations of atomistic or coarse-grained models of entangled polymer systems. We will first present our simulation results for entangled polymer melt which cover the entire range from loosely to tightly entangled polymers. The excellent agreement demonstrates that the tube model can make parameter-free, quantitative predictions for plateau moduli on the basis of a purely topological analysis. Then, we will discuss the extension of the primitive path analysis to strained systems as well as a time-dependent version of our original, time-saving algorithm. By using the time mapping, one can obtain the precise relaxation mudulus from free-end PPA.

DY 12.5　Tue 15:30　H47

The Shape of a Polymer in a Crowded Environment — Viktoria Blavatska[1], •Christian von Ferber[2,3], and Yurij Holovatch[1,4] — [1]Institute for Condensed Matter Physics, Lviv, UA — [2]Applied Mathematics Research Centre, Coventry University, UK — [3]Physikalisches Institut, Universität Freiburg — [4]Institut für Theoretische Physik, Universität Linz, AT

An environment with correlated obstacles may be used to model the crowded environment typically found in a biological cell. Does such a correlated environment change the universal conformations of a polymer in solution? We study the universal characteristics of the shape of a flexible polymer chain in an environment with correlated structural obstacles, with a power law decay x^{-a} of the correlation. To determine the universal behaviour of the polymer shape we apply the field-theoretical renormalization group approach in d dimensions and use the technique of a double expansion in the parameters $\varepsilon = 4 - d$ and $\delta = 4 - a$. The scaling exponents for the polymer are shown to depend on the disorder correlation. Further we estimate universal shape ratios, in particular the size ratio of the end-to-end and gyration radii $\langle R_e^2 \rangle / \langle R_G^2 \rangle$ as well as the averaged asphericity ratio $\hat{A}_d$. The results show that the asymmetry of the polymer shape is increased in crowded correlated environments as compared to the pure solution case.

DY 12.6　Tue 15:45　H47

Molecular Weight Dependence of Polymer Dynamics: A Molecular Dynamics Simulation Study — Andre Bormuth and •Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 6, 64289 Darmstadt

We perform molecular dynamics simulations for an all-atom model of poly(propylene oxide) to study the dependene of polymer melt dynamics on the molecular weight. The main focus is the regime of low molecular weights at the molecule-polymer crossover, i.e., chains comprised of N=2-100 monomers. Our studies include conformational transitions, structural relaxation, and Rouse dynamics. We find that the rates of conformational transitions, apart from weak chain end effects, do not depend on molecular weight and obey an Arrhenius law. However, upon cooling the heterogeneity of conformational dynamics increases and correlated forward-backward jumps, i.e., deviations from Markov behavior, become important. For the structural relaxation, a non-Arrhenius temperature dependence is accompanied by a more spatially heterogeneous nature of dynamics at lower temperatures. Mode-coupling theory captures some aspects of the glassy slow-down, but it does not enable a complete description. The structural relaxation time strongly increases with increasing molecular weight for short chains, while it is independent of chain length for sufficiently long chains N$>$30. The role of deviations from Gaussian chain statistics on the dynamical behavior is discussed.