SYMP 2: Computational soft matter physics

Time: Thursday 14:00–17:00 Location: H 0105

Invited Talk SYMP 2.1 Thu 14:00 H 0105

DNA mechanics and dynamics — •Richard Lavery — Institut de Biologie et Chimie des Protéines, CNRS UMR 5086 / Université de Lyon, France

The DNA double helix is easily deformable, both on a local level, in response to changes in base sequence or to interactions with other species, and on a global level, in response to external constraints such as supercoiling or stretching. We are using molecular mechanics and dynamics to study these properties of DNA and to relate them to the biological behavior of this vital biomacromolecule. Our studies have enabled us both to examine the extreme deformations of the double helix which can be induced during single molecule experiments and the more subtle deformations which are vital in protein-DNA recognition processes. We are also investigating how different base sequences influence DNA dynamics and can impact on processes such as energy transfer.

S.B. Dixit *et al.*, Biophys. J. **89**, 3721 (2005).
E. Emanuele *et al.*, J. Phys. Chem. **109**, 16109 (2005).
R.A. O'Flanagan *et al.*, Bioinformatics **21**, 2254 (2005).
T. Lionnet *et al.*, Phys. Rev. Lett. **96**, 178102 (2006).
F. Lankas *et al.*, Structure **14**, 1527 (2006).

Invited Talk SYMP 2.2 Thu 14:30 H 0105

Charge mobility of discotic mesophases of polyaromatic hydrocarbons: a multiscale quantum/classical study — •Denis Andrienko — MPI for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Discotic liquid crystals form columnar phases, where the molecules stack on top of each other and the columns arrange in a regular lattice. The self-organization into stacks results in the one-dimensional charge transport along the columns. Combining atomistic molecular dynamic simulations, Kinetic Monte Carlo, and Marcus-Hush approaches we study the effect of the side chain substitution on the transition temperatures as well as molecular ordering in the mesophases. Our study rationalizes the differences in charge carrier mobilities in the herringbone and hexagonal mesophases which is predominantly due to the change of the overlap integral between the neighboring molecules. We are able to reproduce the trends and magnitudes of charge mobilities as measured by pulse-radiolysis time-resolved microwave conductivity technique. The proposed multiscale approach can readily be generalized to study conductive properties of conjugated polymers and disordered molecular crystals.

SYMP 2.3 Thu 15:00 H 0105

Viscoelasticity and primitive path analysis of entangled polymer liquids: From f-actin to polyethylene — Nariya Uchida[1], Gary S. Grest[2], and •Ralf Everaers[3] — [1]Department of Physics, Tohoku University, Sendai 980-8578, Japan — [2]Sandia National Laboratories, Albuquerque, NM 87185, USA — [3]Université de Lyon, Laboratoire de Physique, École Normale Supérieure de Lyon, CNRS UMR 5672, 46 allée d'Italie, 69364 Lyon Cedex 07, France

We combine computer simulations and scaling arguments to develop a unified view of polymer entanglement based on the *primitive path analysis* (PPA) of the microscopic topological state. Our results agree with experimentally measured plateau moduli for three different polymer classes over a wide range of reduced polymer densities: (i) semidilute theta solutions of synthetic polymers, (ii) the corresponding dense melts above the glass transition or crystallization temperature, and (iii) solutions of semi-flexible (bio)polymers such as f-actin or suspensions of rodlike viruses. Together these systems cover the entire range from loosely to tightly entangled polymers. In particular, we argue that the primitive path analysis renormalizes a loosely to a tightly entangled system and provide a new explanation of the successful Lin-Noolandi packing conjecture for polymer melts.

R. Everaers *et al.*, *Science 303*, 823-826 (2004)
N. Uchida, G.S. Grest and R. Everaers, *J. Chem. Phys.*, in press.

15 min. break

Invited Talk SYMP 2.4 Thu 15:30 H 0105

Simulation of coarse-grained membrane models — •Marcus Müller — Institut für Theoretische Physik, Georg-August Universität, Göttingen

Collective processes in membranes – like pore formation in membranes under tension or fusion of two apposed bilayers – exhibit a large degree of universality, i.e., similar phenomena are observed in systems that significantly differ in their microscopic interactions. Since these phenomena involve length scales of micrometers and time scales of milliseconds, they are difficult to study by atomistic simulations, but minimal coarse-grained models can provide detailed and direct insights into the molecular mechanisms.

An advantage of coarse-grained models is the calculation of free energies of self-assembled structures. This can be accomplished either by mapping the model onto molecular field theories and using the mean field approximation or by special simulation techniques. In the latter case, applying an external, ordering field, one imposes a pre-defined structure onto the fluid in the disordered phase (e.g., at high temperature). This structure closely resembles the self-assembled structure (at low temperature, in the absence of an ordering field). Subsequently, one gradually switches off the external, ordering field and, in turn, increases the control parameter (temperature) that drives the self-assembly. The free energy difference along this reversible path is obtained via thermodynamic integration or expanded ensemble simulation techniques.

Invited Talk SYMP 2.5 Thu 16:00 H 0105

Fragments of a computational cell: mesoscopic simulations of soft matter — •Julian C. Shillcock — MEMPHYS - Center for Biomembrane Physics, University of Southern Denmark, Odense, Denmark

As computer power increases, it becomes possible to build complex and realistic computational models of cellular processes. Vesicle fusion has recently been intensively studied using a variety of simulation techniques ranging from atomistic Molecular Dynamics to self-consistent field theory. Whereas continuum models of the fusion pathway assume that the membranes pass through known shapes and transitions, simulations allow the membranes to adopt whatever shapes and structures minimise their free energy. Quite distinct techniques, such as Monte Carlo and Molecular Dynamics simulations, have revealed common features in the fusion process, giving confidence that the observed molecular rearrangements are not simply artifacts of the models. Having established that vesicle fusion can be observed in simulations, the next stage is to extend the models to capture more features of biological systems. Computational membrane models are now sophisticated enough to allow the "sculpting"of membranes into crypts or microvilli, to study the diffusion and reactions of particles diffusing within these confined volumes, and to follow the translocation of rigid nanoparticles across a membrane. In the latter process, which may be important for investigating the toxicity of nanomaterials, the shape and interactions of the nanoparticles determine the efficiency of the translocation process. We present results showing that computational models of membranes are not only structurally similar to biological membranes, but can also be used to study dynamic processes such as fusion, endocytosis, invagination, and the interactions of synthetic nanoparticles with membranes.

SYMP 2.6 Thu 16:30 H 0105

Non-cubic bicontinuous space partitions: transformation pathways between cubic lyotropic phases and possible equilibrium structures — •Gerd E Schröder-Turk — Inst. für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen

Triply-periodic minimal surface families that contain the cubic Gyroid (G), Diamond (D) and Primitive (P) surfaces are studied in terms of their global packing and local curvature properties. These properties are central to understanding the formation of mesophases in amphiphile molecular systems. The surfaces investigated are the tetragonal, rhombohedral and hexagonal tD, tP, tG, rG, rPD and H surfaces. These non-cubic surfaces furnish topology-preserving transformation pathways between these cubic surfaces. We introduce 'packing homogeneity', defined as the standard deviation Δd of the distribution of the channel diameter throughout the labyrinth; the channel diameter d is determined from the medial surface skeleton centered within the domains. Curvature homogeneity is defined similarly as the standard de-

viation ΔK of the distribution of Gaussian curvature. We demonstrate that the cubic G and D surfaces are the most homogeneous members of these families. We show that the tetragonal pathway between the cubic phases to be more homogeneous than the rhombohedral one, relevant to pressure-induced phase transitions between these phases. We discuss the possibility of bicontinuous hexagonal equilibrium phases.

SYMP 2.7 Thu 16:45 H 0105

Reproducibility of single particle-dynamics. The Hori-type generalized Langevin equation — •Jörg R. Silbermann[1], Sabine H. L. Klapp[1,2], and Martin Schoen[1] — [1]Stranski-Lab für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin — [2]Institut für Theoretische Physik, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin

We consider the dynamics of a single tagged particle of mass M in a 2D Lennard-Jones (LJ) system. Employing the Mori-Zwanzig projector operator formalism, one can derive [1] an effective equation of motion of the form of a generalized Langevin equation (GLE). The "random force" $F_0^r(t)$ appearing in the GLE is in general unknown. For a harmonic solid, however, one can derive a GLE where $F_0^r(t)$ coincides with the total force $F_0^*(t)$ acting on the tagged particle in a "reference system", where the mass is changed from M to an arbitrary mass m^*. We study to what extent this GLE is still able to capture the dynamics of the tagged particle under conditions where the harmonic approximation is no longer justified. To this end we compute typical time-autocorrelation functions for the tagged particle in molecular dynamics simulations for the full LJ system and compared those with the ones from the GLE. We find excellent agreement at low temperatures and a surprisingly good reproduction of the dynamics even in the high-temperature liquid phase.

[1] K. Wada, J. Hori, Prog. Theor. Phys. **49**, 129, (1973).