CPP 33: Focused Session: Computational Polymer Physics - New Developments (jointly with DY)

Time: Wednesday 14:00–16:45 Location: MOL 213

Invited Talk CPP 33.1 Wed 14:00 MOL 213
Multiscale Simulation of Soft Matter: Challenges — •Florian Müller-Plathe — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Centre of Smart Interfaces, Technische Universität Darmstadt, Germany

Systematic coarse-graining approaches to the simulation of soft materials are now commonplace. Structural coarse-graining can be performed by a variety of methods such as Iterative Boltzmann Inversion and Force Matching. There remain, however, substantial challenges to the coarse-grained models, such as: (i) Dynamical properties. Current structure based coarse-graining methods predict too fast mobilities. (ii) Scale-bridging between particle models (e.g molecular dynamics) and continuum models (e.g. finite elements). (iii) The application of coarse-graining techniques to real-world problems. This lecture will highlight the challenges and survey approaches to overcome them.

Invited Talk CPP 33.2 Wed 14:30 MOL 213
A self-consistent field approach for crosslinked polymer materials — •Friederike Schmid — KOMET 331, Institut fuer Physik, JGU Mainz

The Self-Consistent Field (SCF) theory is one of the most powerful approaches to studying inhomogeneous polymer melts and solutions. It is nowadays a standard method to calculate nanoscale structures at polymer-coated surfaces or at interfaces in polymer mixtures, self-organization of amphiphilic polymers, phase transitions between block copolymer mesophases, to name just a few examples. However, the original SCF theory has a major drawback: It can only treat polymeric fluids. Many polymeric materials have a network structure, which means that they respond elastically to stress and that deformations are restored. In the talk, a generalized SCF theory for networks shall be proposed. As a first application, it is used to study the effect of crosslinking on the order-disorder transition in ordered lamellar block copolymer phases.

Invited Talk CPP 33.3 Wed 15:00 MOL 213
Mechanical separation of short double stranded DNA: Effect of pulling geometry — •Sanjay Kumar — Department of Physics, Banaras Hindu University, Varanasi 221 005, India

Using the Exact Enumeration technique and Molecular Dynamics simulation, we study the influence of force on the melting of DNA. A force is applied perpendicular to the helix direction to study the DNA unzipping. The force-temperature diagram is consistent with the experiment but differs significantly with the theoretical predictions. However, when a force is applied along the helix direction, we have a situation similar to the DNA rupture. We show that the rupture force increases linearly with the chain length and approaches to the asymptotic value. This is consistent with the experiment. We also observed that the rupture force depends logarithmically on the loading rate. It was found that below a certain loading rate, rupture force decreases with temperature, whereas above it, increases with temperature. Using phenomenological argument, we explain why the rupture force has distinctively different behavior for two temperatures above and below a certain loading rate. We substantiate our argument with the simulation.

15 min. break

Invited Talk CPP 33.4 Wed 15:45 MOL 213
Soft coarse-grained models for multi-component polymer melts — •Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität, Göttingen, Germany

The universal equilibrium properties of dense multi-component polymer systems can be described by minimal coarse-grained models that only incorporate the relevant interactions – connectivity along the molecular backbone, limited compressibility of the polymer liquid, and repulsion between unlike segment species – via simple potentials. In such a model an effective segment corresponds to many monomeric repeat units of a chemically realistic representation and the interactions between effective segments are soft. This large degree of coarse-graining allows for a computationally efficient description of large three-dimensional systems characterized by a large invariant degree of polymerization.

I will discuss simulation techniques for studying the structure formation in block copolymer materials and illustrate the advantages and limitations of this coarse-grained description.

Invited Talk CPP 33.5 Wed 16:15 MOL 213
Simulations of Polymer Electrolytes for Lithium-Ion Batteries Highly Accurate Polarizable Potentials — •Grant Smith — University of Utah, Salt Lake City, UT, USA

There is increasing interest in using polymer electrolytes for secondary lithium batteries due to improved safety and mechanical properties compared to conventional electrolytes based on organic solvents. In polymer electrolytes a lithium salt is dissolved in a polymer matrix. In principle molecular dynamics (MD) simulations can provide important insight into the mechanism of Li+ cation coordination and transport in polymer electrolytes, facilitating the development of materials with improved properties. Such simulations require the development of potential energy functions, or force fields, that are able to faithfully reproduce polymer-polymer, salt-polymer and salt-salt interactions. We have developed such potentials based upon high-level quantum chemistry studies of model compounds, and have found that the inclusion of polarization effects is critical in obtaining an accurate description of polymer electrolytes. I will discuss the nature of these potentials as well as insights into polymer electrolytes we have gained through extensive MD simulations utilizing them.