

CPP 12: Modeling and Simulation of Soft Matter II

Time: Monday 15:00–17:15

Location: MER 02

Invited Talk

CPP 12.1 Mon 15:00 MER 02

Adaptive Resolution Simulations: Past, Present and Open (Boundaries) Future — LUIS A. BAPTISTA, MAURICIO SEVILLA, KURT KREMER, and •ROBINSON CORTES-HUERTO — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Soft-matter systems challenge computational methods because interactions spanning a wide range of lengths and time scales require a multiscale approach capable of describing open systems and non-equilibrium conditions. Nonetheless, a high-resolution method is often only necessary to describe a relatively small portion of the system, embedded in a less detailed environment or even a particle reservoir. In this context, the adaptive resolution simulation (AdResS) method provides a seamless interpolation between high- and low-resolution descriptions: both concurrently present within the simulation box in a thermodynamically consistent framework.

In this talk, we introduce the AdResS method and present a few applications as a multiscale simulation protocol. By reducing the complexity of the low-resolution model and describing it as an ideal gas, it is practically possible to control the chemical potential of the system. In this context, we show extensions of AdResS as an efficient method to compute chemical potentials and solvation free energies in complex molecular systems. We also discuss its recent development into an open-boundary method to perform grand canonical and non-equilibrium molecular dynamics simulations. Finally, we examine possible extensions and challenges of developing the method into an open adaptive QM/MM approach.

CPP 12.2 Mon 15:30 MER 02

Chirality propagation across length scales: the case of knots in helical polymers — YANI ZHAO¹, JAN ROTHÖRL², POL BESENIUS³, PETER VIRNAU², and •KOSTAS DAOULAS¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Department of Physics, Johannes Gutenberg University, Mainz, Germany — ³Department of Chemistry, Johannes Gutenberg University, Mainz, Germany

We use computer simulations to investigate the effect of helicity in isolated polymers on the topological chirality of their knots. Polymers are described by worm-like chains (WLC), where chiral coupling between segments promotes helical conformations. The sign and magnitude of the coupling coefficient u determine the sense and strength of helicity. The excluded volume is adjusted via the radius R of a hard sphere placed at each WLC segment. Open and compact helices are, respectively, obtained for R that is zero or smaller than the length of the WLC bond, and R that is a few times larger than the bond length. We perform Monte Carlo sampling of polymer conformations for u spanning a broad range of values, from achiral polymers to polymers with well-developed helices. First, we demonstrate that the coil-helix transition in our model is not a phase transition but a crossover. Next, we perform statistical analysis of knotted polymer conformations and demonstrate that the sense of polymer helicity, left- or right-handed, influences the handedness of molecular knots and identify a generic mechanism that underlies this effect.

CPP 12.3 Mon 15:45 MER 02

Dynamics of the Rouse-mode distribution of a Gaussian chain in an external field and connection to spinodal decomposition — •DAVID STEFFEN¹, JÖRG RÖTTLER², and MARCUS MÜLLER¹ — ¹Institut für Theoretische Physik, Georg-August-Universität, 37077 Göttingen, Germany — ²Department of Physics and Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada

The current description of spinodal decomposition of a homopolymer blend via dynamic self-consistent field theory (D-SCFT) is based on the density of the monomers and uses a time-independent Onsager coefficient. This is sufficient for long wavevectors where the dynamics can be solely described by the diffusion of the center of mass. On small timescales and for larger wavevectors the dynamic is influenced by subdiffusive processes inside the chain. Therefore, a more microscopic description is needed. In this work, we provide an analytical solution for the time-dependent Rouse-mode distribution of a single chain in a weak external field. The time-dependent monomer density can then be obtained via a projection from the Rouse-mode distribution.

Although different Rouse-mode distributions yield the same monomer density, an accurate description of the dynamics of the density requires the more microscopic description via the Rouse-modes distribution. This technique can be extended to the spinodal decomposition of a binary homopolymer melt. We compare the analytical results for the density and the Rouse-mode distribution to Monte-Carlo simulations of Gaussian chains.

CPP 12.4 Mon 16:00 MER 02

Simulation of diblock-copolymer membrane fabrication — •NIKLAS BLAGOJEVIC und MARCUS MÜLLER — Universität Göttingen, Institut für Theoretische Physik

Diblock copolymers can be used to create integral asymmetric membranes used for ultrafiltration purposes – for example water purification. The combination of evaporation-induced self assembly (EISA) and non-solvent induced phase separation (NIPS) is a promising way for efficient membrane fabrication. The importance of different time- and length-scales makes it difficult to investigate the influence of processing parameters and molecular architecture in experiments. We use a coarse-grained particle based model in conjunction with the Single-Chain in Mean Field (SCMF) algorithm to simulate membrane fabrication with EISA and SNIPS to understand how the membrane structure is formed and how it can be tailored by different processing parameters and varying molecular architecture. For example, we find that nonsolvent macrovoids in the membrane substructure coarsen with an increasing distance into the membrane, while an increasing incompatibility between nonsolvent and polymer leads to more narrow and straight macrovoids.

15 min. break

CPP 12.5 Mon 16:30 MER 02

Salt effects on N-isopropylacrylamide in aqueous solutions. Experimental measurements, Kirkwood-Buff theory and computer simulation — JAKUB POLÁK, •DANIEL ONDO, and JAN HEYDA — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, 166 28 Prague 6, Czech Republic

In this work, we investigate salt-specific effects on N-isopropylacrylamide (NiPAM) by means of densimetry and vapor pressure osmometry, employing family of sodium and guanidinium salts from low NiPAM concentration up to the solubility limit. Employing Kirkwood-Buff (KB) theory, complete set of effective pair interactions, KB-integrals, at any composition are determined, serving as a bridge to well calibrated molecular dynamics (MD) simulation. All atom MD simulations were used in direct analogy to the experiments and volumetric properties determined. For the first time, in-silico vapor pressure osmometry experiment was performed and excess osmolality evaluated from ternary solution structure. Finally, we establish a strong correlation between salt effect on NiPAM hydration and the salting-out ability of studied salts.

CPP 12.6 Mon 16:45 MER 02

Evaporation-induced confinement assembly of functional terpolymer microparticles — •ELIAS M. ZIRDEHI¹, MANUEL TRÖMER², ANDRÉ H. GRÖSCHEL², and ARASH NIKOUBASHMAN¹ — ¹Institute of Physics, Johannes Gutenberg University Mainz — ²Institute of Physical Chemistry, University of Münster

Evaporation-induced confinement assembly of terpolymers is an effective technique for fabricating internally structured microparticles (MPs). The wide range of usable building blocks allows for a large variety of MPs, but poses also an immense challenge due to the staggering amount of process parameters, which cannot be explored through experiments alone. Therefore, we performed dissipative particle dynamics simulations of a bead-spring model to study the directed assembly of triblock copolymers in evaporating droplets. We developed a semi-grand canonical simulation approach, where droplet particles in the vapor phase are periodically removed to drive evaporation at constant flux. In this model, the evaporation rate is controlled by the frequency and the number of particle removal. The resulting shrinking of the droplet was in excellent agreement with theory and experiments. We then implemented this procedure to investigate how the final morphology of terpolymer MPs is influenced by the evaporation rate as well

as surfactant type. Finally, the possibility of altering the morphology tailored for specific applications by adding homopolymers will be discussed.

CPP 12.7 Mon 17:00 MER 02

Wavenumber dependent viscosity of a system of particles coupled dissipatively to a Lattice Boltzmann fluid — ●JOYDIP CHAUDHURI¹ and BURKHARD DÜNWEG^{1,2} — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²Department of Chemical and Biological Engineering, Monash University, Clayton, Victoria 3800, Australia

We consider a particle based Molecular Dynamics (MD) system coupled dissipatively to a stochastic Lattice Boltzmann (LB) fluid. The employed force coupling method is dissipative which means that the

velocity of an MD particle is damped with respect to the velocity of the LB fluid interpolated to the position of the particle. The present study explores the viscosity response of such a coupled LBMD system due to a sinusoidally varying external force. The analytic theory for that system is based upon a two-fluid model, whose predictions are well corroborated by numerical tests. Except for the respective viscosities of the two uncoupled fluids, the total viscosity of the coupled system depends on a hydrodynamic screening length associated with the Stokes coupling parameter, the mass density ratio, and the wavenumber of the applied external force. In the asymptotic long-wavelength limit, the total viscosity is just the sum of the two input viscosities. This behavior deviates significantly from the well known Einstein prediction for dilute colloidal dispersions, and this is due to the different type of particle-fluid coupling.