CPP 17: Modeling and Simulation of Soft Matter I

Time: Tuesday 9:30–11:15 Location: H38

Invited Talk CPP 17.1 Tue 9:30 H38

Continuum models for water's peculiar behavior on the nanoscale — •Alexander Schlaich — Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Germany

Water at the nanoscale exhibits unexpected properties relevant to many soft matter applications, ranging from the hydration forces that stabilize biological matter, via interfacial viscous effects that dominate wear behavior, to the unique dielectric behavior. Atomistically, these effects can be linked to the strong hydrogen bonding network and the corresponding water orientation and density at interfaces and in confinement – observables directly accessible from molecular simulations. However, relating these properties to experimental, typically macroscopic or at least averaged quantities is a tedious task. Here I will discuss some of the progress we have made in the last few years in deriving effective descriptions of the microscopic details that can be used to apply continuous descriptions and thereby extract, for example, experimentally accessible hydration pressure, permeance, or capacitance. Our recent work has focused on combining concepts from solid state theory and soft matter physics to accurately treat the electrode/electrolyte interface, and I will present our analysis of the unusually high capacitance of pure water capacitors.

CPP 17.2 Tue 10:00 H38

Coupled self and collective dynamics in highly charged colloidal Yukawa-systems — •Daniel Weidig and Joachim Wagner — University of Rostock, Rostock, Germany

We investigate binary mixtures of highly charged colloidal particles employing Brownian dynamics simulations. In mixtures of identically charged, but differently sized particles solely the Stokes-Einstein diffusion coefficients differ, while the interactions are practically size-independent. Due to these identical interactions the static structure of all species are identical and independent on dynamical properties of the particles, as observed in partial static pair correlation functions. A dynamical coupling of both self and collective motion is observed in these systems. The long-time self-diffusion coefficient of a larger species is enhanced by the presence of a smaller, more mobile species and vice versa. Similar coupling effects are as well observed in the initial correlation decay of partial, distinct intermediate scattering functions, quantified by relaxation rates and stretching exponents of stretched exponentials. For all the here mentioned parameters, in the limit of strongly electrostatically coupled colloidal systems in first approximation linear dependencies on the size-ratio and reduced number density are observed. Despite we investigated highly dilute colloidal suspensions, where normally hydrodynamic interactions are neglectable, we found especially in binary mixtures an enhancement of the self and collective diffusion coefficients due to hydrodynamic interactions. Contrary, in one-component systems, hydrodynamic interactions do not have significant influence on time-dependent diffusion coefficients.

CPP 17.3 Tue 10:15 H38

Grand canonical molecular dynamics simulation of surface-initiated polymerization — •Bhuwan Poudel and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

The post-characterization of polymer brushes prepared from surface-initiated polymerization (SIP) is challenging because of their unique morphology and limitations in experimental techniques. However, in simulation counterparts, it is much easier to gain control over SIP processes. In this work, we used grand canonical molecular dynamics simulations to investigate the growth kinetics and characterization of polymer brushes. The SIP was studied by varying the grafting density. At low grafting densities, nearly monodisperse brushes were obtained. The dispersity was found to be increased with increasing grafting density; as a result, brushes with broad molecular weight distribution were obtained. We also showed that parameters such as thickness, molecular weight, and dispersity can be precisely controlled during SIP. The results suggests that the method presented here provides strategies to synthesize polymer brushes and tailor their properties more efficiently.

CPP 17.4 Tue 10:30 H38

IR Spectroscopy and Electric Field Simulations Enabled by the Atomic Polar Tensor Neural Network — •Philipp Schienbein — Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany

Vibrational spectroscopy is a vital technique for uncovering microscopic structure and dynamics of condensed phase systems. However, interpreting such spectra at the microscopic level often requires theoretical support. While ab initio molecular dynamics (AIMD) has proven effective for this purpose, its high computational cost – especially when using electronic structure methods beyond GGA DFT – can be prohibitive. We have recently introduced a machine learning molecular dynamics (MLMD) approach for accurately calculating IR spectra using the atomic polar tensor, a size-intensive physical observable that can uniquely be defined for each atom and is thus broadly applicable across diverse systems. Notably, the atomic polar tensor also rigorously enables MLMD simulations under external electric fields. In this work, I benchmark this method against explicit AIMD simulations demonstrating comparable accuracy with significantly reduced computational cost and present applications of the atomic polar tensor neural network. These examples highlight its potential to drive novel physical insights, particularly in scenarios requiring large-scale MD simulations or computationally intensive electronic structure methods.

CPP 17.5 Tue 10:45 H38

Reducing dynamical helical polymers to 1D Ising models: long-range effects from polymer self-avoidance — •Keerti Chauhan[1], Marcus Müller[2], and Kostas Daoulas[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Georg-August-Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany

Cooperative chiral order in dynamic helical polymers (DHP) is commonly understood by reducing them to 1D Ising chains. Each spin can switch between $\sigma = -1$ and $\sigma = +1$ to represent rapid interconvertion between left-handed (M) and right-handed (P) helical twist. Spins are ferromagnetically coupled to capture the energetic disadvantage of boundaries between P and M domains. Currently, all 1D Ising models of DHP assume nearest-neighbor (NN) spin-spin interactions. We use a minimal model to challenge this assumption and investigate whether polymer self-avoidance, due to excluded volume, leads to effective non-local coupling between spins. Polymers are represented by freely-jointed chains with reversible hinges and helicity is described by a NN 1D Ising Hamiltonian with coupling strength J. Ideal and self-avoiding DHP are generated via a Monte Carlo scheme. First, we verify that in ideal chains the spins reproduce the statistics of a NN 1D Ising model with coupling strength J. Next, we find that chain self-avoidance does create effective long-range interactions between spins, as demonstrated by spin-spin correlation functions and free-energy calculations. These interactions renormalize J and create finite-size effects that are inconsistent with a NN 1D Ising behavior.

CPP 17.6 Tue 11:00 H38

Stabilization of Sodium Dodecyl Sulfate Reverse Micelles in Acid Solutions and Toluene from Molecular Dynamics Simulations — •Qixuan Li — Ruhr University Bochum, Bochum, Germany

The anionic surfactant Sodium dodecyl sulfate (SDS) forms reverse micelles (RMs) in two non-miscible components above the critical micelle concentration. Although the RMs in salt or alkali solution has been investigated in previous studies, less is known on the working mechanism of acids in SDS RMs. Here, we employ all-atom molecular dynamics simulations using Generalized Amber Force Field (GAFF) to investigate the effects of chloroauric acid (HAuCl4), fluoroboric acid (HBF4), phosphoric acid (H3PO4) and perchloric acid (HClO4) solutions on the stability of the RMs through spontaneous self-assembly in toluene. We find that all kinds of acids can stabilize micellar structure, and in particular high concentration of acids can significantly enhance the stability of RMs. In addition, H2PO4- anions tend to accumulate close to the RM surface, because they can form stable hydrogen bonds with the sulfate-based headgroup of SDS molecules or hydrated protons. Our findings can help to rationalize the impact of different acids on the RMs stability and in turn on the metallic nanoparticles synthesis where the RMs are used as nanoreactors.