

CPP 43: Fluids and Glasses II

Time: Wednesday 15:00–16:00

Location: ZEU 255

CPP 43.1 Wed 15:00 ZEU 255

Chemical Potential Calculation of Dense Fluids using Hamiltonian Adaptive Resolution Simulation — ●MAZIAR HEIDARI, ROBINSON CORTES-HUERTO, KURT KREMER, and RAFFAELLO POTESIO — Max Planck Institute for Polymer Research, Mainz, Germany

The calculation of chemical potential of fluids is a relevant and challenging problem in computational chemistry and physics. Here, we propose a method which employs the recently multi-scale Hamiltonian Adaptive Resolution Simulation (H-AdResS) method to calculate the chemical potential of dense fluids. In H-AdResS, the simulation domain is subdivided in regions of high and low resolutions, coupled through a hybrid region. Since the dynamics of particles are obtained from a global Hamiltonian, the generated statistical ensembles of the system are well-defined. In our method, the fluid within the high resolution region is coupled with an ideal gas of non-interacting particles, and to enforce a uniform density profile an external force is computed on-the-fly and applied. Then the converged compensation forces are integrated across the hybrid region to obtain the Gibbs free energy difference between the two resolutions. The resulting Gibbs free energy is related to the excess chemical potential of the fluid with respect to the ideal gas. We validated this method by calculating the excess chemical potentials of fluid mixtures.

CPP 43.2 Wed 15:15 ZEU 255

A Refined Polarizable Water Model for the Coarse-Grained MARTINI Force Field — ●JULIAN MICHALOWSKY¹, LARS SCHÄFER², JOHANNES ZEMAN¹, CHRISTIAN HOLM¹, and JENS SMIAŁEK¹ — ¹Institute for Computational Physics, University of Stuttgart, Allmandring 3, D-70569 Stuttgart, Germany — ²Center for Theoretical Chemistry, Faculty of Chemistry and Biochemistry, Ruhr-University, Universitätsstraße 150, D-44780 Bochum, Germany

We propose a refined version of the polarizable MARTINI water model designed for the use with long-range electrostatics. Our new model improves the resemblance of the experimentally measured water mass density at room temperature and matches the experimentally measured dielectric constant of water. Our investigations show that the new model performs stably with a variety of commonly used sets of simulation parameters, remaining fully applicable within a reaction field framework. The oil/water partitioning behavior of uncharged MARTINI beads is thoroughly investigated: Lennard-Jones interactions between our new model and the remaining MARTINI beads are tuned to reproduce the hydration free energies obtained with the original polarizable water model. The cross-interactions with charged bead types are matched to the experimentally observed area per lipid of a solvated dipalmitoylphosphatidylcholine (DPPC) lipid bilayer. We additionally analyzed the potentials of mean force between different sample pairs solvated in the refined polarizable water model and compared the results to reference data obtained using the original water

model and atomistic approaches.

CPP 43.3 Wed 15:30 ZEU 255

Diverging time scale in the dimensional crossover for liquids in strong confinement — ●SUVENDU MANDAL and THOMAS FRANOSCH — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Technikerstr. 21A, A-6020 Innsbruck, Austria

We study a strongly interacting dense hard-sphere system confined between two parallel plates by event-driven molecular dynamics simulations to address the fundamental question of the nature of the 3D to 2D crossover. As the fluid becomes more and more confined the dynamics of the transverse and lateral degrees of freedom decouple, which is accompanied by a diverging time scale separating 2D from 3D behavior. Relying on the time-correlation function of the transversal kinetic energy the scaling behavior and its density-dependence is explored. Surprisingly, our simulations reveal that its time-dependence becomes purely exponential such that memory effects can be ignored. We rationalize our findings quantitatively in terms of an analytic theory which becomes exact in the limit of strong confinement.

CPP 43.4 Wed 15:45 ZEU 255

Structure, Dynamics and Phase Behavior of a Discotic Liquid Crystal Confined in Nanoporous Anodic Aluminum Oxide Membranes — ●ARDA YILDIRIM¹, KATHRIN SENTKER², PATRICK HUBER², and ANDREAS SCHÖNHALS¹ — ¹Bundesanstalt für Materialforschung und -prüfung [BAM] — ²Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg (TUHH)

Discotic liquid crystals (DLCs) are a promising class of soft matter for electronic applications. This is due to their ability to organize and stack themselves into columns in a hexagonal columnar mesophase, driven by the overlapping of the π -orbitals of their aromatic core. This leads to a high charge-carrier mobility along the column axis. Previous studies on DLCs showed that their properties, such as phase transition temperatures and enthalpies, are susceptible to nanoconfinement [1,2]. In this study, 2,3,6,7,10,11 hexakis[hexyloxy] triphenylene (HAT6), a triphenylene based DLC, was confined into parallel aligned cylindrical nanopores of anodic aluminum oxide (AAO) membranes by melt infiltration in the isotropic phase under an argon atmosphere. Furthermore, the pore surfaces of a series of membranes were chemically modified, resulting in a more hydrophobic pore surface than the unmodified ones. The structure, dynamics, and the phase behavior of HAT6 confined into modified and unmodified nanopores of AAO were investigated by broadband dielectric spectroscopy and differential scanning calorimetry. Results will be discussed in detail.

[1] C. Krause and A. Schönhals, *J. Phys. Chem. C*, 2013, 117, 19712.

[2] C. Krause et al., *Colloid Polym. Sci.*, 2014, 292, 1949.