CPP 24: Complex Fluids and Colloids IV (joint session BP/CPP/DY, organized by DY)

Time: Tuesday 14:00–15:15 Location: H46

CPP 24.1 Tue 14:00 H46

Rheo-Chaos of Frictional Grains — •Matthias Grob, Annette Zippelius, and Claus Heussinger — Institut für Theoretische Physik, Georg-August Universität, Göttingen, Deutschland

A two-dimensional dense fluid of frictional grains is shown to exhibit time-chaotic, spatially heterogeneous flow in a range of stress values, σ, chosen in the unstable region of s-shaped flow curves. Stress controlled simulations reveal a phase diagram with reentrant stationary flow for small and large stress σ. In between no steady flow state can be reached, instead the system either jams or displays time dependent heterogeneous strain rates $\dot{\gamma}(\mathbf{r},t)$. The results of simulations are in agreement with the stability analysis of a simple hydrodynamic model, coupling stress and microstructure which we tentatively associate with the frictional contact network.

CPP 24.2 Tue 14:15 H46

From classical to quantum and back: A Hamiltonian scheme for adaptive multi-resolution classical/path integral simulations — •Karsten Kreis[1,2], Mark E. Tuckerman[3,4,5], Davide Donadio[1,6], Kurt Kremer[1], and Raffaello Potestio[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Department of Chemistry, New York University (NYU), New York, NY 10003, USA — [4]Courant Institute of Mathematical Sciences, NYU, New York, NY 10012, USA — [5]NYU-East China Normal University Center for Computational Chemistry at NYU Shanghai, Shanghai 200062, China — [6]Department of Chemistry, University of California Davis, One Shields Ave., Davis, CA 95616, USA

Quantum delocalization of atomic nuclei affects the physical properties of many hydrogen-rich liquids and biological systems. To accurately model these effects, Feynman's path integral formulation of quantum statistical mechanics is typically employed, which implies a substantial increase in computational overhead. By restricting the quantum description to a small spatial region, this cost can be significantly reduced. Herein, we derive and validate a rigorous, Hamiltonian-based scheme that allows molecules to change from quantum to classical and vice versa on the fly as they diffuse through the system, both reducing overhead and making quantum grand-canonical simulations possible. Our adaptive resolution approach paves the way to efficient quantum simulations of biomolecules, membranes, and interfaces.

CPP 24.3 Tue 14:30 H46

All-Atom and Coarse-Grained Molecular Dynamics Simulation of Ionic Liquids — •Tamisra Pal and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstrasse 6, 64289 Darmstadt

Room temperature Ionic Liquids (RTILs) have garnered much interest in the last few years as they possess tremendous potential for application in industry as reaction media. The high complexity of these liquids originating from their self-assembly or nano-scale aggregate formation motivates us to understand more on their dynamics. We have employed molecular dynamics simulation for RTILs to connect the length and time scales of simulation models with different levels of molecular resolution provided by the mapping scheme. Specifically, we have investigated a coarse grained (CG) model of 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][PF_6]) and its all-atom (AA) description, at various temperatures. In this way, we unravel the different dynamical modes associated with dynamic heterogeneity and structural relaxation and we quantitatively compare the characteristic time scales from the two model systems to ascertain the effects of coarse graining on the dynamical behavior. The spatial and temporal aspects of molecular dynamics have been studied via calculating non-Gaussian parameters, particle displacement distributions, overlap functions and dynamic susceptibilities. Our simulation results provide a microscopic understanding to the presence of "fast" and "slow" moving particles contributing to dynamic heterogeneity and their relevance for the structural relaxation of ionic liquids.

CPP 24.4 Tue 14:45 H46

Equilibrium interfacial free energies and Turnbull coefficient for bcc crystallizing colloidal charged sphere suspensions — •Thomas Palberg[1], Patrick Wette[2,3], and Dieter M. Herlach[2] — [1]Institut f. Physik, Johannes Gutenberg Universität, 55099 Mainz, Germany — [2]Institut f. Materialphysik im Weltraum, DLR, 51147 Köln, Germany — [3]Space Administration, DLR, 53227 Bonn, Germany

The interfacial free energy (IFE) is a central quantity in crystallization from the meta-stable melt. In suspensions of charged colloidal spheres, nucleation and growth kinetics can be accurately measured from optical experiments. We here re-analyze the strictly linear increase of previously reported CNT-effective non-equilibrium IFEs estimated from such experimentsutilizing classical nucleation theory (CNT). For five aqueous suspensions of charged spheres and one binary mixture, we utilize a simple extrapolation scheme and interpret our findings in view of Turnbull's empirical rule. Our first estimates for the reduced equilibrium IFE, $\sigma_{0,bcc}$, between coexisting fluid and bcc-crystal phases are on the order of a few k_BT. Their values are not correlated to any of the electrostatic interaction parameters but rather show a systematic decrease with increasing size polydispersity and a lower value for the mixture as compared to the pure components. At the same time, σ_0 shows an approximately linear correlation to the entropy of freezing. The equilibrium interfacial free energy of strictly monodisperse charged spheres may therefore be still greater.

CPP 24.5 Tue 15:00 H46

Size matters: can we use a Hamiltonian adaptive resolution scheme to simulate an open system? — •Robinson Cortes-Huerto, Maziar Heidari, and Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz, Germany

Finite size effects are ubiquitous in molecular dynamics simulations. Apart from the obvious implicit size effects due to periodic boundary conditions, explicit size effects are consequence of simulating a fixed and relatively small number of particles. In particular, measurements of density fluctuations within a sub-domain of a periodic simulation box are strongly dependent on the sub-domain size. These effects can be neglected by carrying out computer simulations for extremely large systems. An alternative solution is to use the Hamiltonian adaptive resolution scheme (H-AdResS), where the computational cost reduces substantially by embedding a relatively small high resolution portion of the system in a larger region at low resolution. Our main goal is to explore the viability to perform grand canonical simulations using this dual-resolution approach. In particular, we propose to use H-AdResS to calculate thermodynamic properties of prototypical molecular liquids in an effective open boundary simulation framework. To this end, we calculate Kirkwood-Buff integrals that connect radial distribution functions, available from molecular dynamics simulations, to thermodynamic properties such as the isothermal compressibility. We compare these results with measurements performed in the fully atomistic case and assess whether an adaptive resolution simulation reproduces the behaviour expected from an open simulation setup.