

CPP 20: Poster: Computational Soft Matter Physics

Time: Tuesday 18:00–20:00

Location: P2

CPP 20.1 Tue 18:00 P2

Solvent effects on linear polymer chains - A Monte Carlo Study — ●CHRISTOPH JENTZSCH^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²TU-Dresden, Institut für theoretische Physik, Germany

In Computer simulations the solvent is usually introduced implicitly by effective attraction between the monomers to reduce computational time. Strong monomer-monomer attractions such as necessary to simulate chain collapse lead to artefacts both in lattice and off-lattice models. Using a high-performance implementation of the Bond-Fluctuation-Method solvent particles can be explicitly taken into account. This allows us to study effects of poor solvent and collapse transitions of individual chains both statically and dynamically. We present results for single polymer chains under thermal solvent conditions as well as the effect of an external force on the conformation statistics of individual chains.

CPP 20.2 Tue 18:00 P2

Parallel Monte Carlo simulation of lattice polymers on graphics processing units — ●MARCO WERNER^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²Technische Universität Dresden - Institut für Theoretische Physik

A parallel version of the bond fluctuation model (BFM) was developed for programmable graphics processing units (GPUs). The BFM is a lattice-based dynamical Monte Carlo method addressing the universal dynamic and static properties of polymer structures [I. Carmesin, K. Kremer, *Macromolecules*, 21, 2819, (1988)]. Recent developments by graphic card industry give rise to new possibilities in terms of system size and simulation speed accessible by the BFM. Modern GPUs provide several hundreds of parallel processors which work most efficient with massively parallel processes. We make use of this architecture by associating each monomer to one parallel process. In one elementary step all monomers are tried to move simultaneously. Hereby, the number of random memory accesses is reduced and the rate of tried moves per monomer increases with increasing number of monomers. The statics and dynamics of samples like polymer melts are compared between parallel and serial BFM-code to ensure the equivalence both methods. On the latest generation of GPU we obtain a maximum up-speed of about 50 compared to actual serial processors.

CPP 20.3 Tue 18:00 P2

Possibility of Coherent Delocalized Nuclear Quantum States

of Protons in Li₂NH — ●OLE SCHÜTT¹, GUILLERMO A. LUDUEÑA², and DANIEL SEBASTIANI¹ — ¹Physics Department, Freie Universität Berlin, Arnimallee 14, 141965 Berlin, Germany — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

We analyze the possibility of quantum delocalization in lithium imide (Li₂NH) in the condensed phase using *ab initio* path-integral molecular dynamics. Our results provide evidence that the effective potential felt by the protons in the material has a toroidal shape. The virtually flat potential may lead to quantum delocalization of the NH protons over the torus.

CPP 20.4 Tue 18:00 P2

Stochastic optimization of capping potentials for mixed QM/MM calculations — ●CHRISTOPH SCHIFFMANN and DANIEL SEBASTIANI — Freie Universität Berlin, Institut für Theoretische Physik, Arnimallee 14, 14195 Berlin

We present a stochastic scheme to design & optimize capping potentials for use at the QM/MM boundary in mixed *ab initio*-classical calculations. In our scheme, the terminal atoms in the quantum subsystem are replaced by optimized capping pseudopotentials. Our aim is to minimize the perturbations in the electronic structure due to the cleaving of covalent bonds across the QM/MM boundary.

Komin, S.; Sebastiani, D. *JCTC* **2009**, 5, 1490-1498
Schiffmann C.; Sebastiani D. (*submitted*)

CPP 20.5 Tue 18:00 P2

Friction contribution to water-bond breakage kinetics — ●YANN VON HANSEN¹, FELIX SEDLMEIER¹, MICHAEL HINCZEWSKI^{1,2}, and ROLAND R. NETZ¹ — ¹Physik Department, Technische Universität München, 85748 Garching, Germany — ²Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742, USA

Based on separation trajectories between water molecule pairs from MD simulations, we investigate the bond breakage dynamics in bulk water. From the spectrum of mean first-passage times, the Fokker-Planck equation allows us to derive the diffusivity profile along the separation coordinate and thus to unambiguously disentangle the effects of free energy and local friction on the separation kinetics. For tightly coordinated water the friction is six times higher than in bulk, which can be interpreted in terms of a dominant reaction path that involves additional orthogonal coordinates.