

CPP 16: Poster: Modelling and Simulation of Soft Matter

Time: Monday 18:30–21:00

Location: P1C

CPP 16.1 Mon 18:30 P1C

Kinetic properties of liquid crystals from coarse-grained and atomistic molecular dynamics simulations — ●SVENJA WÖRNER, JOSEPH RUDZINSKI, KURT KREMER, and TRISTAN BERAU — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Liquid crystals display liquid-like behavior while maintaining a long-range crystalline order, giving rise to unique material properties. To understand macroscopic processes, e.g. phase transitions, large systems need to be studied on time scales not accessible by atomistic models. Coarse grained models make these sizes and time scales accessible.

In this work we investigate the liquid crystal mesogen 8AB8, containing a stiff, photoisomerizable azobenzene core with flexible alkyl tails. Mukherjee et al. have previously developed a coarse-grained model of 8AB8, which displays the correct thermodynamic and structural properties. Not only is it able to form a smectic phase, the model also reproduces the transition temperature of the disordered to smectic phase transition of the underlying atomistic model. Reducing the degrees of freedom usually leads to a non-trivial modification of the timescales for different processes sampled by the coarse-grained model. Two well-characterized translocation pathways in the smectic A phase are studied in detail, utilizing a Markov state model framework to systematically assess the differences in the transport kinetics between the coarse-grained and atomistic models. Investigating the precise source of the discrepancies between the two models implicates an approach for reparametrization of the coarse-grained model.

CPP 16.2 Mon 18:30 P1C

Systematic Reduction of Chemical Compound Space using Coarse-Graining and Clustering Algorithms — ●KIRAN KANEKAL, KURT KREMER, and TRISTAN BERAU — Max Planck Institute for Polymer Research

The size of chemical compound space is prohibitively large for the fast generation of hypersurfaces that define structure-property relationships, which are necessary for implementing inverse molecular design. In this work, we use a dataset consisting of all small organic molecules with up to 8 heavy atoms (i.e. excluding hydrogen atoms) as an initial proxy for the entire chemical compound space. This relatively small slice of the total space consists of ~100,000 molecules. We demonstrate a reduction of this space in two steps. First, we apply the AutoMartini algorithm developed by Berau and Kremer to systematically determine a coarse-grained representation for each molecule in the dataset. We subsequently cluster molecules by using similarity measures corresponding to specific chemical and structural descriptors. We then assess the extent to which the initial chemical compound space was reduced and whether the diversity of the space is sufficiently reflected in its coarse-grained counterpart. The resolution of the coarse-grained space can then be tuned either by introducing new bead types or by reducing the number of atoms assigned to a bead. This framework will provide a means for efficient high throughput sampling of chemical compound space (as highlighted by Menichetti and coworkers in their work).

CPP 16.3 Mon 18:30 P1C

Sampling of chemical space via high-throughput molecular dynamics simulations — ●ROBERTO MENICHETTI, KURT KREMER, and TRISTAN BERAU — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The increasing request for new materials with tunable physical and chemical properties requires a rational optimization of molecular structures. An exhaustive characterization of all compounds is clearly unfeasible in practice, due to the overwhelming size of chemical space. Instead, we introduce a stochastic Monte Carlo importance sampling approach, in which thermodynamic properties are computed, at every step, by means of high-throughput molecular dynamics simulations. Though chemically heterogeneous, the resulting ensemble of molecules optimizes the target property of interest. In this work, we describe our methodology and apply it to the case of the free energy of insertion of a compound in a phospholipid membrane.

CPP 16.4 Mon 18:30 P1C

Dynamics of Seeded A β 40-Fibril Growth from Atomistic

Molecular Dynamics Simulations: Kinetic Trapping and Reduced Water Mobility in the Locking Step — ●NADINE SCHWIERZ¹, CHRISTINA V. FROST², PHILLIP L. GEISSLER¹, and MARTIN ZACHARIAS² — ¹Chemistry Department, University of California, Berkeley, California 94720, United States — ²Physik Department, Technische Universität München, 85748 Garching, Germany

Filamentous β -amyloid aggregates are crucial for the pathology of Alzheimer's disease. Despite the tremendous biomedical importance, the molecular pathway of growth propagation is not completely understood and remains challenging to investigate by simulations due to the long time scales involved. Here, we apply extensive all-atom molecular dynamics simulations in explicit water to obtain free energy profiles and kinetic information from position-dependent diffusion profiles for different A β fibril growth processes. Our approach provides insight into the molecular steps and allows close agreement with experimental binding free energies and macroscopic growth rates. Water plays a decisive role, and solvent entropy is identified as the main driving force for assembly. Fibril growth is disfavored energetically due to cancellation of direct peptide-peptide interactions and solvation effects. The kinetics of growth is consistent with the characteristic dock/lock mechanism, and docking is at least 2 orders of magnitude faster. In the locking step, the dynamics is much slower due to kinetically trapped conformations and the reduced mobility of hydration water.

CPP 16.5 Mon 18:30 P1C

DPD study of Polymer Ring Brushes — ●MARTIN JEHSER^{1,2} and CHRISTOS N. LIKOS² — ¹Department of Physical Chemistry, University of Vienna, Austria — ²Faculty of Physics, University of Vienna, Austria

Recently, experimental methods have been developed allowing the production of well defined surface-grafted polymer nanoparticle systems without free chain-ends [1], i.e., grafted polymer loops or rings. In the present investigation, equivalent situations are studied making use of computer simulations based on Dissipative Particle Dynamics [2,3] (DPD) a highly efficient, coarse grained, method smoothly covering the range from several nanometers up to the mesoscale region. In order to reproduce the behaviour of adsorbed polymers in addition to the conservative forces an attractive interaction between one (or in case of loops both) chain end(s) and a surface, represented by a soft wall, are introduced as well. Aim of the study is the comparison of properties of loops and rings to those of trails as functions of surface coverage free chain concentration and particle distance.

The results show that with increasing grafting density, loops and rings become more and more rodlike in structure and increase the layer thickness in the same way as linear chains do. A rise in concentration of free polymer chains results into a compression of the brush.

[1] R. Rotzoll, P. Vana, *Journal of Polymer Science Part A: Polymer Chemistry* 46, 7656 (2008) [2] R.D. Groot, P.B. Warren, *J. Chem. Phys.* 107, 4423 (1997) [3] M.M. Nardai, G. Zifferer, *J. Chem. Phys.* 131, 124903 (2009)

CPP 16.6 Mon 18:30 P1C

Application of molecular dynamics simulations to the elastoplastic model — ●LAWRENCE SMITH and ANDREAS HEUER — Institute of Physical Chemistry, WWU Münster, Germany

We are studying the rheology of amorphous solids through the coupling of minimal systems in the athermal limit. This ansatz is based on an existing elastoplastic model [1] while reducing the abstraction by using real molecular dynamics (MD) simulations as microscopic states.

For the microscopic systems, a well investigated Lennard-Jones model of $N=130$ particles is employed. This size approximately corresponds to the number of particles known to participate in a plastic rearrangement. Multiple instances of this system are arranged on a lattice and interact during plastic events by distributing shear stresses. This distribution follows the standard elastic propagator $\cos(4\theta)/r^2$.

We study the relevant ingredients of this model to identify plasticity during running MD simulations. Of key interest are the impact of the coupling on stress drop distributions and spatial correlations of plasticity as well as on the behaviour of the system during row.

[1] Nicolas, A., Martens, K. and Barrat, J. L. *EPL* 107, 44003 (2014)