CPP 28: Modeling and Simulation of Soft Matter III

Time: Wednesday 15:00–16:00 Location: H34

CPP 28.1 Wed 15:00 H34

Many-body potentials and optimized mapping schemes for systematic coarse-graining of small conjugated molecules — •Sayan Dutta[1,2,3], Muhammad Nawaz Qaisrani[4], Denis Andrienko[4], and Arash Nikoubashman[1,2,3] — [1]Johannes Gutenberg-Universität, Mainz, Germany — [2]Leibniz-Institut für Polymerforschung, Dresden, Germany — [3]Technische Universität Dresden, Dresden, Germany — [4]Max-Planck Institut für Polymerforschung, Mainz, Germany

Bottom-up coarse-graining approaches frequently focus on reproducing structural order parameters, ensuring consistency with structural properties from the underlying atomistic model. However, these methods often struggle to predict thermodynamic quantities accurately, leading to challenges in transferability. Furthermore, the coarse-grained (CG) potential is typically highly sensitive to the mapping scheme, introducing representability issues. Recent CG models increasingly enhance traditional pair potentials by incorporating a potential that depends on the local density around each CG particle, which effectively includes many-body interactions in a mean-field approximation. We introduce local density dependent potentials based framework in the CG forcefield for small conjugated molecules, which are widely used in the field of organic photovoltaic materials. Our framework captures the local density around each mapped CG site to ensure structural and thermodynamic accuracy, while enhancing computational efficiency compared to its atomistic counterparts.

CPP 28.2 Wed 15:15 H34

Simulation of the fabrication of integral asymmetric polymer membranes using continuum modeling — •Gregor Häfner and Marcus Müller — University of Göttingen, Germany

Integral asymmetric polymer membranes represent a promising class of functional macromolecular systems with a wide range of potential applications, including water purification and protein separation. Their synthesis is achieved through a two-step procedure: (i) the controlled self-assembly of diblock copolymers upon solvent evaporation, to form a cylindrical morphology that is oriented perpendicular to the solution-gas interface. (ii) a solvent-non-solvent exchange, raising the polymer concentration above its glass transition, thereby freezing the matrix phase while allowing the entry of the non-solvent through the cylindrical minority domains. Below, the non-solvent macrophase separates from the polymer to form a porous sub-structure.

In order to gain insight into the physical processes, we perform computer simulations. A continuum model is employed which treats the local concentrations as order parameters and minimizes a free-energy functional. In the limit of high viscosity, the dynamics are purely diffusive, enabling comparison with a particle-based model. We use the continuum model to optimize the final membrane morphology and identifying optimal parameter regions and dependencies. Additionally, this model enables the treatment of finite viscosities. We demonstrate that in the presence of a bariocentric flow, the frozen top layer can be transported downwards to prevent the formation of macro voids beneath the isoporous top layer.

CPP 28.3 Wed 15:30 H34

Highways in pore networks — •Werner Napetschnig[1], Ekaterina Baikova[1,2], Maximilian Fuchs[1,2], and Karin Zojer[1,2] — [1]Institute for Solid State Physics, Graz University of Technology, Austria — [2]Christian Doppler Laboratory for Mass Transport through Paper

When simulating Stokes flow of gases through porous media, the volume flow is often explained by microstructural properties. However, most of these properties do not adequately account for the arrangement of pathways, which is strongly material dependent. Here, we highlight the importance of considering these pathways and explore different techniques to identify flow paths. A pore network model based on micro-computed tomography scans of paper samples serves as the basis for air flow simulation. Two methods are evaluated to identify transport pathways and locate the most critical flow regions. In the first method, the maximum flow rate between individual pores determines the paths. It is shown that the highest flow rate travels between fiber network layers and clusters at a few exit pores. The second method identifies paths iteratively through a stochastic approach where the flow rate is the weighting factor. We identified the most frequently used highway regions. In addition, we studied the orientation and geometric properties of these highways. Our results show that only a few segments within the highways significantly influence the overall flow. Therefore, these highways need to be numerically represented when defining the explanatory microstructure properties.

CPP 28.4 Wed 15:45 H34

A lattice Boltzmann study of bijels as a novel type of catalyst support structure — •Johannes Martinus Peter Beunen and Jens Harting — Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien, Cauerstraße 1, 91058 Erlangen, Germany

Due to their high surface area to volume ratio porous media are very suitable as catalyst support materials. However, the stochastic morphology of commercially available supports generally results in poor reaction product transport and inefficient use of the therein-contained catalyst material. These issues can be alleviated by making use of catalyst supports acquired from spinodally derived architectures due to their beneficial percolation properties. In particular, architectures obtained from bicontinuous interfacially jammed emulsion gels (bijels) seem to provide a viable route to manufacture stable catalyst supports that resolve the aforementioned issues. In this work, this type of porous support is further investigated by means of the three-dimensional lattice Boltzmann method. First, we simulate the formation of bijels by an extension of the lattice Boltzmann method, to allow for multicomponent fluids and particles with non-neutral wetting properties. We report on the improved properties of the resulting porous structures compared to stochastic equivalents for usage in chemical reactors. Hereafter, the lattice Boltzmann method is employed again to further validate the enhanced performance of bijel-derived geometries by means of reactive flow simulations. Our findings suggest that bijel-derived catalyst support structures allow for an almost threefold increase in reactor effectiveness.