**Soft-core approach to modeling morphology and transport in proton exchange polyelectrolyte membranes**

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Soft-core simulations, in particular dissipative particle dynamics (DPD), become increasingly popular in modeling of nanostructured materials. In DPD, large molecules are dissected into quasiparticles that interact with each other through “soft” repulsive short-range potentials. This approach provides a superb computational efficiency and expands simulation spatial and temporal scales. The price to pay is crudeness of the models that limits their applicability and predictive capacity.

            The talk describes author's effort to increase predictive capabilities of DPD, targeting a class of very complex systems: proton exchange polyelectrolytes. The efforts include advancing parameterization of potentials, inclusion of electrostatic interactions, and finally, inclusion of a proton model that artificially mimics Grotthius hopping mechanism. At each stage, the methodology is validated against experimental data on reference systems. Finally, DPD is applied to morphology and transport in two well-known PEM: sulfonated polystyrene (the hydrophilic subphase of sPS-based block copolymer membranes for fuel cells) and Nafion.

            Despite the crudeness of the model, simulation results qualitatively, and in many respects quantitatively, predict the specifics of nanoscale segregation and transport in the hydrated PEM, including water diffusion and proton conductivity. The limitations of the approach are especially visible at low hydration and related to the model particle size. Overall, the proposed model opens up an opportunity to study self-assembly and water and proton transport in polyelectrolytes using computationally efficient DPD simulations, and, with further refinement, it may become a practical tool for theory informed design and optimization of perm-selective and ion-conducting membranes with improved properties.