Molecular Simulation of Phase Separation and Transport in Nafion Membranes

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We used MD simulations to study microstructure and transport in Nafion membranes solvated in water, methanol, and water-methanol mixtures. Special attention was paid to the conformations of sidechains. We found that the sidechain in all solvents is quite stiff and forms strong hydrogen bonds with the solvent molecules. Specifics of solvation in water and methanol are discussed. The results of MD simulations are in reasonable agreement with the experimental density and diffusion coefficients.

We observed a pronounced phase separation with formation of hydrophilic clusters dispersed in the hydrophobic matrix. The water clusters form a random network. As the degree of solvation increased, we observed the formation of water clusters containing up to ca. 100 water molecules. In contrast to the conventional network models, the water clusters do not form a continuous hydrophilic subphase. The cluster size distribution is rather wide and evolves in time due to formation and break-up of temporary bridges between the clusters. This dynamic behavior of the cluster system allows for the macroscopic transfer of water and counterion. The calculated diffusion coefficients of water are in reasonable agreement with experimental data.

We will discuss mesoscale simulation of phase separation using coarse grained lattice models and density functional theory.

References.

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