Proton conduction through Nafion-like membranes

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The conduction of a proton and its deuterium and tritium isotopes through a model Nafion-like membrane is explored. This conduction has potential applications for fuel cells and isotope separation technologies. The dissociative water potential model of Mahadevan and Garofalini is an atomistic potential. It is used to model hydrogen-hydrogen, oxygen-oxygen and oxygen hydrogen interactions. This allows for the formation of hydronium and zundel species. This potential reproduces room-temperature properties of water, such as structure, cohesive energy, diffusion constant, and vibrational spectrum. [1] The potential also includes a temperature and pressure dependant short-range O-H repulsions to account for the density changes at higher temperatures holding pressure constant at 1atm and high-pressure data at select temperatures.[1] A three-dimensional, atomistic extension of the Nafion potential surface model proposed by Paddison, Paul, and Zawodzinski is considered to treat water/sulfonate and proton/sulfonate interactions.[2]

The proton isotope conduction will first be considered classically through molecular dynamics and Monte Carlo methods. Our long term goal is to include quantum treatment of the proton using the method of Gomez and Peart.[3] Comparing isotope effects with experiment will be a first test of the model.

(1) T. S. Mahadevan, and S. H. Garofalini, "Dissociative Water Potential for Molecular Dynamics Simulations," J. Phys. Chem. **111**, 8919 (2007).
(2) S. J. Paddison, R. Paul, and T. A. Jr. Zawodzinski, "Proton friction and diffusion coefficients in hydrated polymer electrolyte membranes: Computations with a non-equilibrium statistical mechanical model," J. Chem. Phys. **115**:16, 7753 (2001).
(3) M. A. Gomez, and P. Peart, "Including quantum subsystem character within classical equilibrium simulations," J. Chem. Phys. **125**, 034105 (2006).