Atomistic Simulation of Proton Transport in Model PEM Pores

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Proton transport in fuel cell membranes such as Nafion or PEEK takes place in a strongly inhomogeneous aqueous environment. Local proton motion, both the magnitude of the transport coefficients and the nature of the transport (vehicle vs. structural diffusion), is influenced strongly by key system properties such as

- the chemical and electrostatic nature of sulfonate groups, and their arrangement on the polymer chains,
- high proton concentration,
- the amount of water in the membrane and thus the nature, size and connectivity of aqueous domains.

Transport coefficients and mechanistic insight obtained from classical molecular dynamics studies employing a simplified empirical valence bond model in simple model pores will be discussed [1-3]. In particular the question will be addressed how the relative importance of Grotthuss (structural diffusion) changes with water content, temperature and sulfonate density.

[1] Spohr, E; Commer P; Kornyshev, AA: Enhancing Proton Mobilitz in Polymer Electrolyte Membranes: Lessons from Molecular Dynamics Simulation, *J. Phys. Chem. B*, **106** 10560-10569 (2002).

[2] Commer, P; Cherstvy, A; Spohr, E; Kornyshev, AA: The nature of water content effect on the proton transport in polymer electrolyte membranes, *Fuel Cells*, **2** 127-136 (2002).

[3]Commer P; Hartnig, C; Seeliger, D; Spohr, E: Modeling of Proton Transfer in Polymer Electrolyte membranes on Different Time and Length Scales, *Mol. Simulation*, **30**, 755-763 (2004).