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Molecular-Dynamics Modeling of Nafion Membranes for Redox Flow Batteries.

Abstract

Nafion is a commonly used polyelectrolyte membrane (PEM) in fuel cells and flow batteries. Nanocomposites of Nafion are used to enhance temperature resistance and proton conductivity. We will present and discuss the novel molecular-dynamics simulations for Nafion films of different thicknesses confined between two potential walls of variable wettability, mimicking the nanofiller surfaces [1-3]. The water cluster sizes showed an increase with film thickness for the high wettability cases, in agreement with SAXS experiments. The in-plane water diffusion was considerably enhanced for the high wettability walls.

The annealing of polymer electrolyte membranes is known to affect the membrane structure and proton conductivity. The observed changes depend drastically upon the annealing temperatures and cooling rates. Our simulations [4] show the compression of hydrophobic Nafion domains by larger water clusters, with a strong antiplasticization effect upon hydration, demonstrated by increasing the glass-transition temperature. The water clusters in hydrated Nafion become more disconnected and larger in size with slower cooling rates / increased annealing time. This results in the decrease of water and hydronium diffusivity and the corresponding conductivity, thereby explaining qualitatively the experimental observations.

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[2]. S. Sengupta and A. V. Lyulin, Molecular Dynamics Simulations of Substrate Hydrophilicity and Confinement Effects in Capped Nafion Films, J. Phys. Chem. B, 122, 6107-6119, 2018.

[3]. S. Sengupta, AV Lyulin, G. Kritikos, K. Karatasos, A. Venkatnathan, R. Pant, P. Komarov, Multiscale modeling examples: new polyelectrolyte nanocomposite membranes for perspective fuel cells and flow batteries , in "Theory and Modeling of Polymer Nanocomposites, V. Ginzburg, L. Hall, Eds, Chapter 6, Springer series in Mater. Sci., 2021.

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