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Experimental and modeling study of blended membranes for direct methanol fuel cells

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Abstract

The dynamics of hydronium ions and methanol molecules in hydrated SPAES and blend membranes are investigated via molecular dynamics simulations using the COMPASS force field. In addition to calculating the diffusion coefficients as a function of the hydration level, an amorphous cell with a specific composition of H_2O molecules and H_3O^+ determined from the experimental data is constructed and tested. The water and methanol diffusion coefficients are considerably smaller at lower hydration levels and room temperature. The diffusion coefficient of the water and methanol molecules increases with increases in the hydration level, and this is in good agreement with experiment data. Analysis of the pair correlation functions supports the experimental observations of the membrane performance with hydration related to the water and methanol diffusion behavior in hydrated SPAES and blend membranes.