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Water desalination and biofuel dehydration through a thin membrane of polymer of intrinsic microporosity: atomistic simulation study

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ABSTRACT: Polymers of intrinsic microporosity (PIMs) have emerged as a special class of polymeric materials and received considerable interest for many potential applications. Nevertheless, most current studies for PIMs are largely focused on gas separation. In this study, we report a simulation protocol to construct a thin membrane of PIM-1, examine its swelling in water and ethanol/water mixture, and explore its performance for water desalination via reverse osmosis as well as biofuel dehydration via pervaporation. The predicted density of the PIM-1 membrane matches well with experimental data. The estimated gravimetric and volumetric swelling degrees are in accord with measured values. As ethanol has a greater capability than water to swell the membrane, the void distribution of the membrane is found to shift to a larger size in ethanol/water mixture than in water. For water desalination, the membrane exhibits water permeability of 8.6×10^{-7} kg·m/(m^2·h·bar) and 100% salt rejection, which is higher than commercial reverse osmosis membranes. For the dehydration of ethanol/water mixture, water permeability and separation factor are 5×10^{-5} kg·m/(m^2·h·bar) and 25, respectively, surpassing poly(vinyl alcohol) and polybenzimidazole membranes. This simulation study provides microscopic insights into the structural and separation properties of PIM-1 membrane from the bottom-up, and suggests that PIM-1 membrane might be an interesting candidate for water desalination and biofuel dehydration.

Keywords: *PIM, water desalination, biofuel dehydration, reverse osmosis, pervaporation, atomistic simulation*

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