Saturating Narrow Pores with Water Enhances the Selectivity of Membrane Separations

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We report atomistic molecular simulation results for the transport of various gases, including methane, H2S, and ethane, through narrow pores saturated by liquid water. The slit-shaped pores are of width of approximately 1 nm. This pore width is selected because the pore surface strongly affects the structure of confined water throughout the entire pore volume. Different solid materials are chosen for the pores, because they are known to affect differently the structure of interfacial water. While some materials are realistic, e.g., the cristobalite mineral of silicon dioxide, others are model ones used as proof of concept in our calculations. Equilibrium molecular dynamics simulations are used to assess the adsorption of various gases within the confined water as a function of bulk pressure. The results show that when confined water is characterized by relatively high fluctuations in density, the solubility of hydrophobic gases can be significantly enhanced compared to the solubility of the same gases in bulk water at comparable thermodynamic conditions. We analysed the free energy barriers experienced by the various gases to enter the pores saturated with water by conducting umbrella-sampling simulations, and we find that the density of water near the pore entrance determines such barriers. We then analysed the transport of the various gases within the pores using a number of statistical techniques, and we compared the selective transport of various gases through the pores filled with water. The results suggest that water could be used to enhance selectivity in membrane separations, although the permeability is reduced significantly compared to values achievable for the pores without water present.