Molecular dynamics simulation of transport and separation of aqueous solutions in model nanopores CRAIG MARTENS, JACOB GOLD-SMITH, University of California, Irvine, RAMSAY BROWN, University of Southern California — We present non-equilibrium molecular dynamics simulations of transport of water and aqueous solutions through model nanopores induced by a pressure gradient. We treat simple model systems consisting of pores through rigid ice-like membranes and pores based on carbon nanotubes with surface charge patterns. The TIP3P water model is employed in the simulations presented. The flux of water and ions through the pores are determined as a function of pore size, surface characteristics, and pressure difference across the membrane. We find that flow rates are significantly higher for the hydrophobic systems for a given pore diameter and pressure gradient, in agreement with recent experiment. For aqueous salt solutions, the phenomenon of ion rejection is quantified as a function of pore size and the nature of the surface. It is found that bipolar charged pores, where positive and negative surface charge regions meet at a sharp boundary, can reject ions virtually completely for pore sizes that show no rejection based on size alone. The ultimate goal of this research is to develop rational design principles at the molecular scale for nanoscale separation and purification.

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