Confined diffusion of monovalent electrolytes

Alfredo Dominguez and Tricia D. Shepherd
Dept. of Chemistry, St. Edward's University, Austin TX

The behavior of monovalent electrolytes in confined aqueous environments is of significant interest in order to advance the knowledge of biological ion channels and material applications involving nanomembranes. In this work, molecular dynamics simulations were employed to investigate the diffusion patterns of monovalent electrolytes through a cylindrical carbon nanotube. Using LAMMPS, MD simulations were performed to a system composed of an atomistic carbon nanopore with coarse-grained water and ions solvents. It was determined that narrow cylindrical pathways act as ion filters dictating the diffusion of specific electrolytes through porous carbon membranes based on the radii size of the nanopore. Based on the results, it is suggested that the ion selectivity of carbon nanotubes can be accomplished by varying the radii size in order to enhance the “hydrophobic gating” effect that can arise in continuous water-filled pores.