

Solute diffusion in cylindrical nanopores

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The behavior of nanoconfined systems is of significant interest to many disciplines, including biophysics, microfluidics, and nanotechnology. We are investigating the influence of a polymer brush surface on solute transport within confined nano-cylindrical spaces. Simulations were performed using Molecular Dynamics (LAMMPS) and a coarse-grained model representing water, solute and monomer particles, with solute concentration, grafting density, and hydrophobicity of the polymer chains being the variables in study. Comparisons to polymer-free nanopore systems are presented. Understanding the aspects of aqueous nanoconfined systems is essential for the engineering and optimization of new materials and processes.