

Abstract Submitted
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Diffusion

Through Tubular Nanotubes DIVYA NARAYAN ELUMALAI, Louisiana Tech University, HERVIN MONLOUIS, Grambling State University, PEDRO DEROSA, Louisiana Tech University and Grambling State University — Nanotubes exhibit exceptional properties that make them promising candidates for many applications that require the transport, storage and/or delivery of fluids, through nanotubes. In order to efficiently plan potential applications, transport properties and interactions such as adsorption, diffusion, and solvent interactions must be understood. Our study focuses on the mechanisms that inhibit or encourage diffusion through these nanostructures and the nature of the interactions responsible for movement of any sort in these regimes. As a specific case we study diffusion through tubular nanotubes. This work treats each interaction individually and aims at successfully modeling the diffusion of particles through the nanotubes as a function of the interaction between the diffusing particles and the nanotube walls. To conduct this research we have employed Monte Carlo calculations, implementing a specific forced random walk algorithm. Preliminary results suggest that any delay in diffusion occurs due to a strong molecule-wall interaction. We believe this is due to the columbic attraction between the diffusing particles and the wall.

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