Water transport through carbon nanotubes with defects

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Understanding the transport of water through hydrophobic channels is vital to the understanding of proteins in biological systems and systems involving carbon nanotubes. By using a carbon nanotube, we can observe similar properties within more complex systems like pore structure within cells. Although, these systems have been studied using carbon nanotubes both through molecular dynamics and experimentally, there are few studies done on water transport through carbon nanotubes with defects. It is important to see how defects can affect the diffusion of water through these hydrophobic channels since they are prevalent in synthesized carbon nanotubes and can occur in biological systems. Throughout this investigation, we utilized LAMMPS in order to perform molecular dynamic simulations with an atomistic carbon nanotube and coarse-grained water model (mW) in order to observe the diffusion of water through carbon nanotubes with defects. Preliminary results indicate that the diffusion of water through hydrophobic carbon nanotubes decreases as the number of defects increases. These observations are depicted by the diffusion coefficients tabulated based on the mean squared displacement of the water atoms in the nanotube.