Molecular dynamics study on the diffusion behavior of water inside functionalized carbon nanotubes

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Carbon nanotubes (CNTs) are considered feasible materials for desalination and wastewater treatment. However, it is reported that functionalized CNTs can change water flux and ion selectivity [1-2]. Therefore, it is of great importance to compare the diffusion behavior of water inside pristine CNTs to that of water inside functionalized CNTs. In this work, we utilize positively charged CNTs (with $-COO^-$) and negatively charged CNTs (with $-NH_3^+$). Detailed investigations are carried out on the systems of rigid (6, 6), (7, 7), (8, 8), (9, 9), and (10, 10) armchair carbon nanotubes, both pristine and functionalized, solvated with Lennard-Jones water fluids. We also compare different water models such as TIP5P and SPC/E to better mimic the interaction between water molecule and CNTs. Self-diffusivity statistics, molecule configurations and hydrogen bonding are computed or examined. It is found that water molecules will have more ordered structure in functionalized CNTs. In small (6,6) CNT, hydrogen bonds tend to aggregate water into a wire and lead to rapid collective drift. Functionalization of CNTs can stabilize the hydrogen bond of water molecules and enhance its lifetime. In (7,7) nanotubes and beyond, hydrogen bonding network allows the water to form regional concentrated clusters. This allows water fluid in extremely low density exhibit rather slow self-diffusion motion. Functionalization can accelerate the oriented motions of water molecules. This fundamental study attempts to provide insights into understanding nanoscale delivery system in aqueous solution.

References

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