The effect of vacancy defects on ion transfer in carbon nanotubes

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Carbon nanotubes are analogues for many biological systems including protein channels through which ions and water flow in a confined space. Experimentally, carbon nanotubes harbor inherent defects, such as vacancies, which may impact computational predictions. We performed large-scale molecular dynamics simulations with a coarse-grained molecular model to investigate the effect of defects on ion flow in order to better model these biological systems. In this study we investigated the relationship between the percent of vacancies for nanotubes of different radii and observed the impact on water coordination, ion hydration, and diffusion coefficients. These results will be useful in assessing the differences between the impact of structural purity of the nanotube and confinement on solution properties.