Coarse-grained simulations of confined water in nanotubes

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Water-filled nanotubes can serve as a model to better understand ion, water, or other solute diffusion through membranes in biological systems. We performed coarse-grained molecular dynamics simulations in order to investigate larger system sizes and longer simulation times possible for common atomistic models. In this work, we studied the impact of different interactions between the nanotube walls and coarse-grained water. By varying the hydrophilic attraction of the wall, we observed changes in flow rates of water through the nanotube. The results of this experiment help us understand how changing the nature of the interactions of water with the nanotube walls impacts the dynamics and the structure of confined water.