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Chirality Effects on Water Transport through Single-Walled Carbon Nanotubes CHANG WON, SONY JOSEPH, NARAYAN ALURU, Department of Mechanical Science and Engineering University of Illinois at Urbana-Champaign — Using quantum partial charges, computed from 6-31G**/B3LYP density functional theory (DFT), in molecular dynamics (MD) simulations, we found that water inside (6,6) and (10,0) single-walled carbon nanotubes (SWCNTs) with similar diameters but with different chiralities has remarkably different structural and dynamical properties. The quantum partial charges, which capture the molecular electrostatic potential, induce relatively stronger wall-water electrostatic interactions at the ends of the tube and weaker electrostatic interactions at the center. The partial charges at the ends of a (10,0) tube are around 4.5 times higher than those of a (6,6) tube. Molecular dynamics simulations with the partial charges show different water dipole orientations. The water diffusion coefficient is found to increase in the presence of the partial charges. From PMF analysis, we found that a larger energy fluctuation inside the partially charged (10,0) tube induces a slower diffusion coefficient when compared with the partially charged (6,6) tube.

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