

Abstract Submitted
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The effects of external electric field on the structure of water inside and outside single-walled carbon nanotubes¹ ZHEN XU, GUO-HUI HU, ZHE-WEI ZHOU — In the present work, all-atom molecular dynamics (MD) simulations are utilized to examine the structure of water inside and outside the armchair SWCNT in the presence of external electric field parallel or perpendicular to the tube axis. Extensive MD simulations have been performed in wide ranges of E (0-3V/nm) at room conditions (300 K and 1 bar). The dependence of liquid density profile, orientation of dipole moment and hydrogen bonds profiles are discussed on the electric fields. With the parallel electric field, the structure of water outside the SWCNT changes slightly while inside the SWCNT the water structure is found to be more ordered. With the perpendicular electric field, the structure of water both inside and outside the SWCNT has changed dramatically. When the strength of field is above 1V/nm, the chains or the layers structures inside the SWCNT are broken and even the isolated water molecule is found. Outside the SWCNT, liquid density profiles, orientation of dipole moment and hydrogen bonds profiles are found to be the non-axisymmetric. This work may be helpful in understanding the physics of the confined water and in the design of future nanofluidic devices.

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