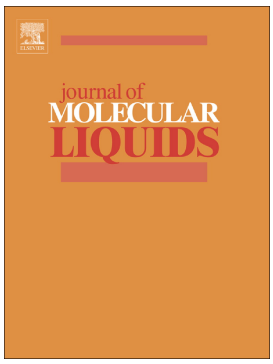

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Structure and Kinetics of Water in Highly Confined Conditions: A Molecular Dynamics Simulation Study

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Abstract

In this work, we carried out a systematic and detailed study of water under severely confined conditions, based on atomistic molecular dynamics (MD) simulations. Specifically, MD simulations were performed for water confined in single-walled capped carbon nanotubes of chiral indices between (4,4) and (10,10). The structure and dynamics of confined water, and its dependence on the diameter and length of the capped carbon nanotubes (CCNTs) was examined, alongside with the influence of the latter on water immersion. Our results show that the axial water density decreases with increasing distance from the open face of the CCNTs, and that water forms well-defined shells along the radius of the CCNTs. The confined water molecules closer to the water–wall interfacial region tend to orient themselves pointing their OH bonds towards the wall. This trend becomes less evident in the inner regions of the CCNTs, so that the water molecules in the central region of the (10,10) CCNT are almost randomly oriented. On the other hand, the water molecules inside the (6,6) CCNT form a single-file chain along the CCNT's axis. Furthermore, the average number of hydrogen bonds per water molecule decreases with increasing length of the CCNT and decreasing diameter. Hydrogen bonding and water orientations in the CCNTs significantly affect the mobility of water, being the mobility of water faster in the (7,7) CCNT than in other CCNTs of the same length.

Keywords: `Capped carbon nanotubes, Water structure and diffusion, Hydrogen bonding, Molecular dynamics simulations`

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