Article

Supplementary Information for Effect of size and temperature on water dynamics inside the carbon nanotubes studied by molecular dynamics simulation.

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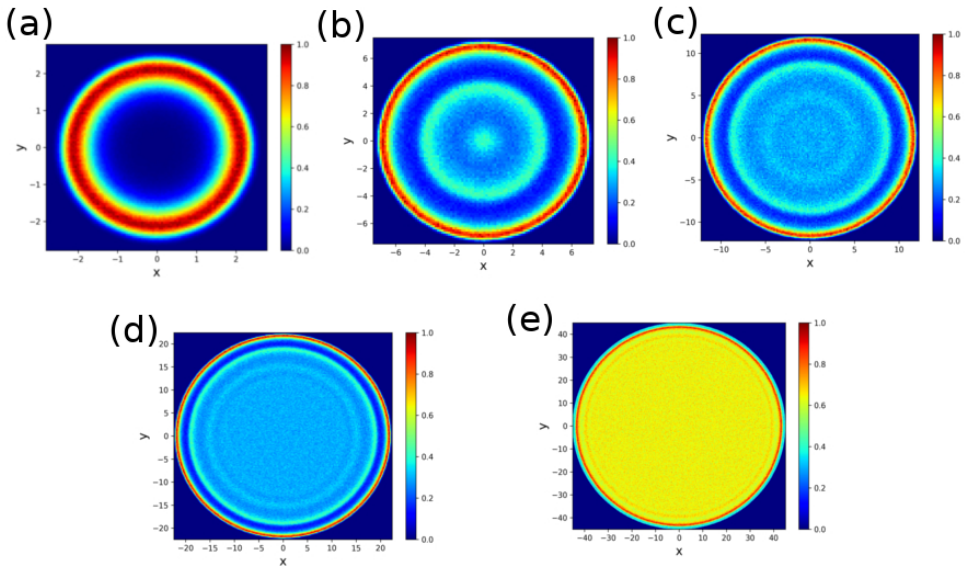

Fig. S1. Density map of water inside various nanotube sizes, shown on the xy plan (a) 1.0 nm, (b) 2.0 nm, (c) 3.0 nm, (d) 5.0 nm, and (e) 10 nm. High water densities are represented in red color, while low water densities tend to have dark blue color.

Citation: . *Preprints* , , .

Received:
Accepted:
Published:

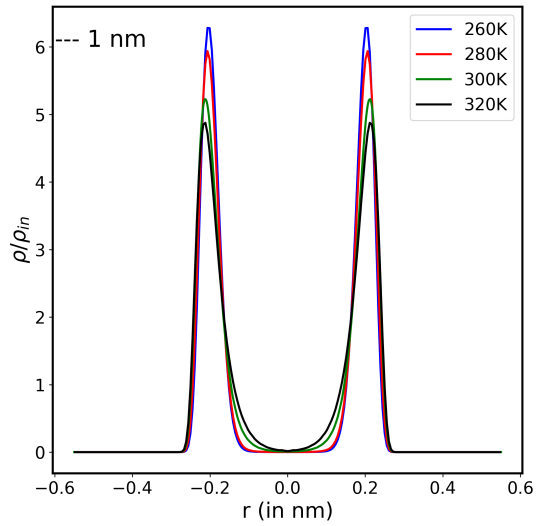

Fig. S2. Radial water local density inside CNT size 1.0 nm at different temperatures. The *x* axis shows the inner diameter of CNT, whereas zero represents the center of nanotube.

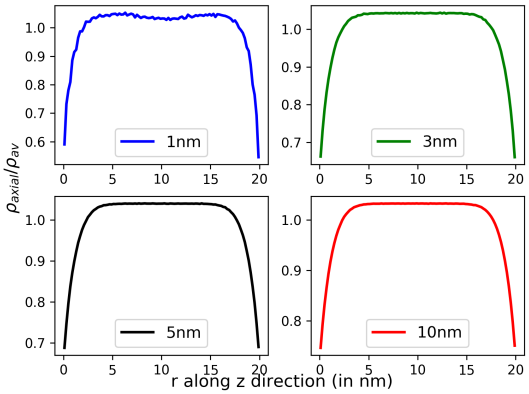

Fig. S3. Axial water density inside different CNT sizes at room temperature. The *x* axis represents the length of CNT in nm.

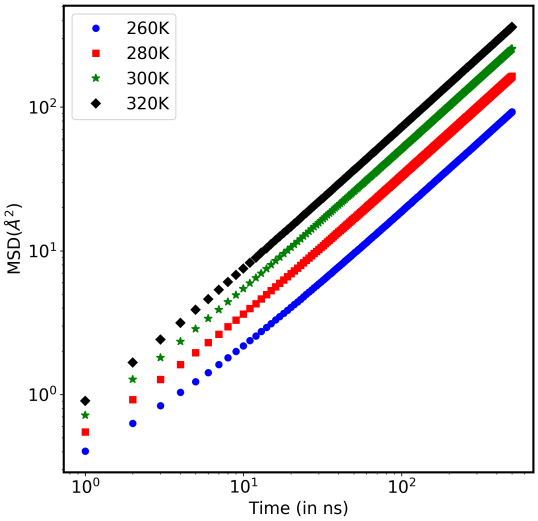

Fig. S4. Mean square displacement (MSD) as a function of time for water inside 3.0 nm CNT, at various temperatures.

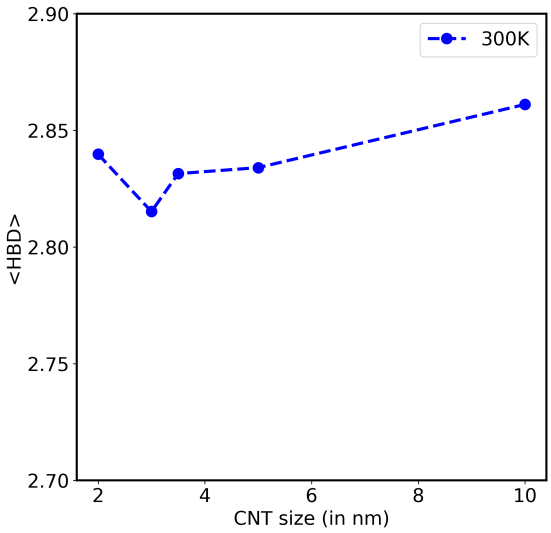

Fig. S5. Average number of hydrogen bonds per water molecule in the inner shell versus different CNT sizes at 300K.