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Molecular dynamics simulation of water conduction within carbon nanotube

ZHOU Yi & DONG ShunLe*

Department of Physics, Ocean University of China, Qingdao 266100, China

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Water molecule transportation through a single-walled carbon nanotube under a charge influence on tube was simulated. As the charge located at middle tube increases from 0.0e to 0.7e, water molecular orientations develop from a consistent orientation ($0 \leqslant q \leqslant 0.4e$) to bipolar orientations (L defect, when $q \geqslant 0.5e$). Water molecule permeation through the channel is almost the same as in charge-free nanotube when $q \leqslant 0.2e$. As q increases further the permeation decreases sharply. When $q=0.6e$ the permeation becomes negligible and the tube channel effectively closes.

molecule dynamics, carbon nanotube, water conduction

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Water transportation through nanoscale channel is important not only in the medical industry but also in basic biological process and it has been studied theoretically and experimentally over years [1]. However, until now it is still difficult to explain about its mechanism. Molecular dynamics (MD) simulation can show us a micro-picture about the transportation in such a nanochannel and give us the information about relevant configurations and permeation characteristics. Recently, more computational studies have been done and offered some structure and dynamics properties of water in nanoscale channel, such as a single-walled carbon nanotube (SWCNT). Hummer et al. first demonstrated that a short carbon nanotube (CNT) could be spontaneously a single file for water molecules and could be modeled as a biological channel. Despite CNT hydrophobic nature they revealed water conduction inside the nanotube at a fast speed [2]. CNT has various outstanding potentials for technical applications in making nanoscale sensors, devices and machines [3–5] or microscopic filters [6].

In this work, we performed MD simulations for a short SWCNT submerging in water. Our SWCNT is (6,6) armchair, 1.35 nm in length and 0.81 nm in diameter. Two graphite sheets are embedded vertically at two ends of this tube. Figure 1 shows that two equal positive charges are put

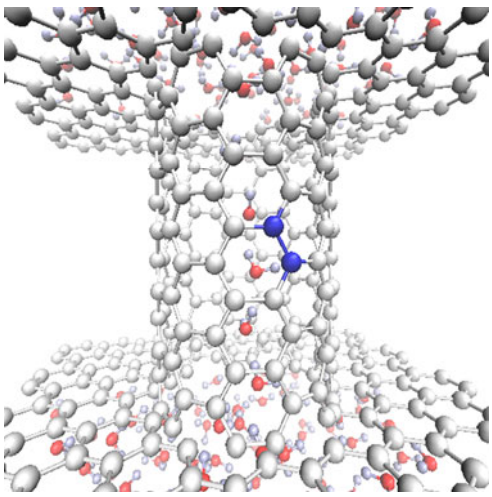

Figure 1 Snapshot of the simulation system. The silver balls are the carbon atoms and the purple balls are two carbon atoms that each carries half positive charges (0.0e, 0.05e, 0.1e, 0.15e, 0.2e, 0.25e. 0.3e and 0.35e). Grey and red are hydrogen and oxygen in water molecule, respectively.

*Corresponding author (email: shunle2001@yahoo.com)

on two carbon atoms around the middle of this SWCNT. Using these two positive charges ensures their total charge center locating exactly at the middle of the nanotube. SWCNT modified by a charge acts as a biological channel such as an aquaporin (AQP) which has the irregular surfaces with inhomogeneous charge distributions [7]. AQPs act as membrane channel proteins and are abundantly present in nearly all life forms [8]. Recently, MD simulations have disclosed that water molecules in the AQPs channels adopt a bipolar orientation due to electrostatic induction, which leads to the exclusion of proton conduction in AQPs channels [9]. Here, we change the charge magnitude, but not its distribution [10,11] to investigate its influence on both water molecular orientation and conduction.

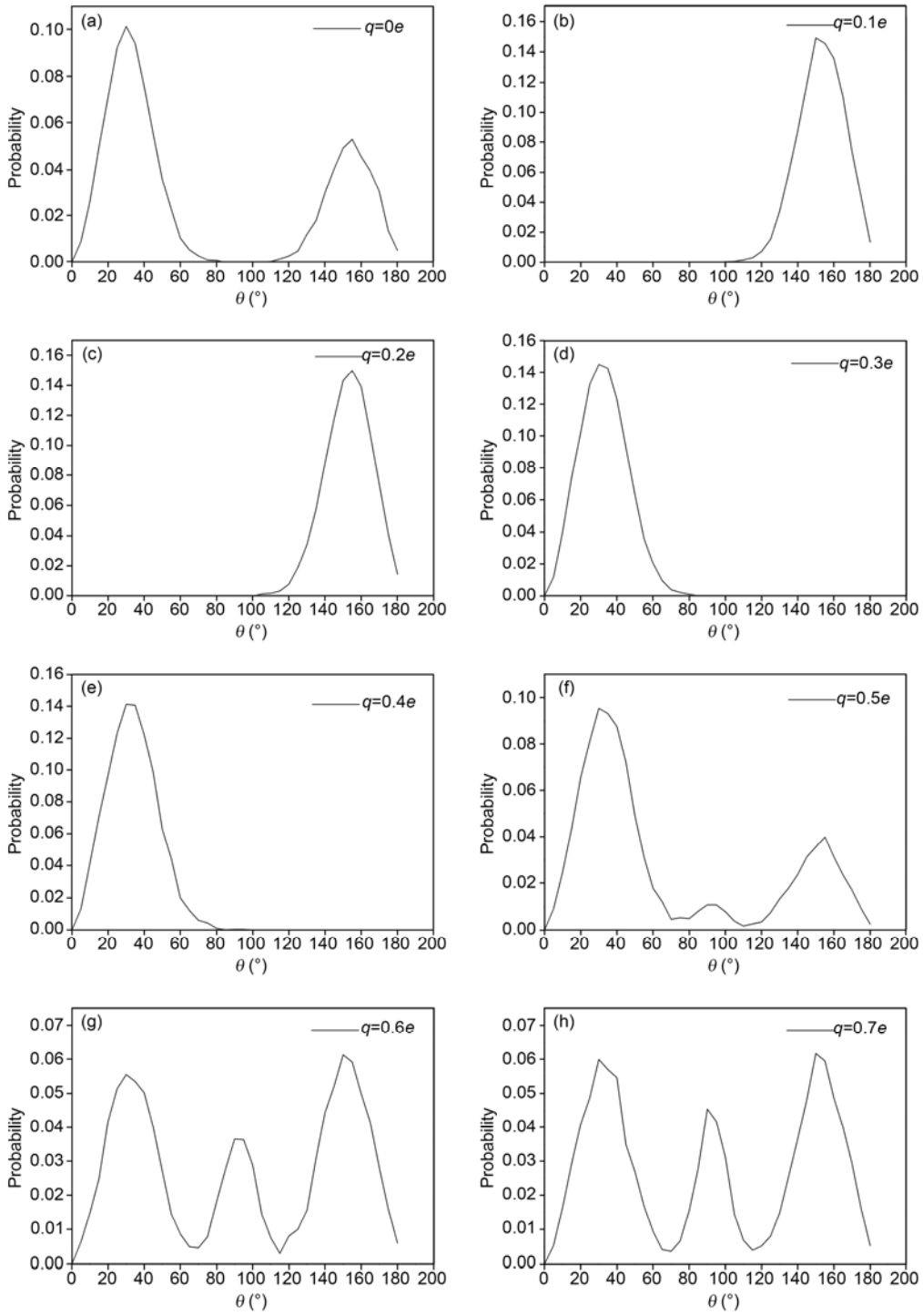

Figure 2 Averaged orientation distributions of the water dipole moments inside the nanochannel for different magnitudes of charges.

1 Methods

During our MD simulations three-site classic potential TIP3P water model [12] was used to describe water intermolecular interaction and rigid water molecular model was adopted, i.e. the OH bond was set at 0.9572 nm and the H–O–H angle at 104.52°. The parameters for carbon atoms were those of type CA in the CHARMM27 force field [13]. Carbon atoms in nanotube and graphite sheets were fixed. The initial box size was L_x=2.5 nm, L_y=2.5 nm, L_z=3.4 nm and periodic boundary conditions were applied in all dimensions. During the simulation the system temperature and pressure were maintained at 300 K and 1 bar, respectively [14]. Lennard-Jones potential parameters ε_{co}=0.103184 kcal/mol and σ_{co}=0.335 nm were obtained by $\varepsilon_{co}=(\varepsilon_{cc}\varepsilon_{oo})^{1/2}$ and $\sigma_{co}=(\sigma_{cc}+\sigma_{oo})/2$ (ε_{cc}=0.07 kcal/mol, ε_{oo}=0.1521 kcal/mol and σ_{oo}=0.3150574 nm, σ_{cc}=0.355 nm). The simulations were carried out with Fortran code NAMD 2.8. Electronic interaction was calculated by particle mesh Ewald method with a cutoff of 1.2 nm and time step was 1 fs, and configurations were stored each 1 ps. A run of 20 ps was needed for equilibration and runs of 2 ns were for collecting data to analyze. A molecular graphics program VMD 1.9 was used for analysis and visualization.

2 Results and discussion

Figure 2 shows the orientation distributions of the water dipole moments within the nanochannel under different magnitudes of the charges. Here θ is the angle between water dipole moment and the tube axis. When total charge q=0.0e, there are two peaks located at 30° and 150°. This is due to that the water molecules pass through nanotube in two directions (sometime leftward and sometime rightward). In Figure 2(b)–(e) only a single peak at θ=30° or θ=150° could be found for q=0.1e, 0.2e, 0.3e and 0.4e and it means that water dipole moments are ordered under the $q\neq 0$ effect. This shows that all water molecules within the nanotube are aligned at a concerted direction during all time (Figure 3(a)) and the reason is that under charge absorption water dipole moment cannot turn over. As q increases to 0.5e, 0.6e and 0.7e, three peaks appear. Except the two peaks at θ=30° and θ=150°, the third peak at about 90° is relevant to L defect [15]. L defect appears when water molecules exhibit opposite orientations in the two halves of the tube, as shown in Figure 3(b). Due to positive q absorbing oxygen, the water molecule at middle tube will be perpendicular to the tube axis and the water molecules in two half tubes will point oppositely. Thus bipolar orientations will be formed (Figure 3(b)). When q increases from 0.5e to 0.6e, the peak at θ=90° increases sharply and this indicates that water molecules are strongly adsorbed by q. The structure of bipolar orientations is of important value because similar water orientations are found in APQ channels [8].

Figure 4 shows the permeation of water molecules through the nanochannel under different charge magnitudes. Here the permeation is defined as the total number of water molecules entering one end of the nanotube and leaving another end per nanosecond. It is easily found that the charge has strong effect on water permeation and the permeation decreases from 10 ns^{-1} to almost 0 when it increases from 0.0e up to 0.7e. When q varies within 0.2e its effect is not obvious. As it increases further the permeation decreases sharply. When the total q is larger than 0.6e the permeation may be negligible and nanochannel is almost closed. This might have implications in novel molecular switch design and biological water channels on the on-off gating mechanism [9].

3 Conclusion

In summary, we have studied the charge effect on water molecule orientation and conduction within nanochannel. The simulation results show that when q is less than (or equal to) 0.2e, the water permeation is almost the same as in charge-free nanotube. The permeation decreases as the

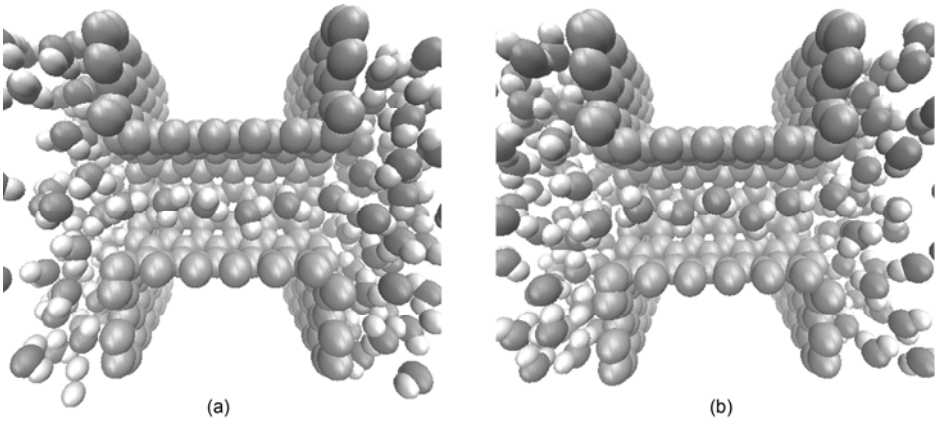

Figure 3 Water orientations within the tube. (a) Concerted orientation; (b) bipolar orientations (L defect).

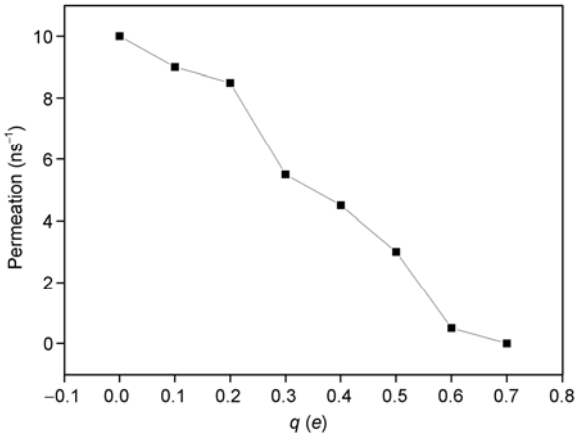

Figure 4 Permeation of water molecules through the nanochannel versus the magnitude of the charge q.

charge further increases until the permeation becomes negligible and the channel effectively closes when $q \geqslant 0.6e$. This indicates the water conduction is sensitive to the charge on nanotube. Therefore, thus carbon nanotube can be treated as an effective controllable on-off gate for water molecules. We found that the bipolar orientations started to set up (L defect) when q was equal to $0.4e$. As q increases to $0.5e$, water orientation at θ=90° increases sharply and the bipolar orientation will be formed completely until q=$0.6e$.

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