



LETTER

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Unexpected effect of an empty cavity on water transport through a combined carbon nanotube

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Abstract – Controlling water transport via an empty cavity can achieve unexpected properties for various applications. In this paper, water transport through a combined carbon nanotube with an empty cavity is studied by molecular dynamics simulations. It is found that the occupancy of water molecules and the transfer rate of water molecules through the combined carbon nanotube can be affected by the size of the cavity unexpectedly under a relatively low pressure difference. The occupancy of water molecules in the combined carbon nanotube and the average transfer rate begin to decrease significantly if the size of the cavity reaches a critical radius of 0.733 nm. The energy gap between water molecules and the combined carbon nanotube is adopted to explain the effect of the empty cavity on water properties in the combined carbon nanotube. Our findings may pave a way for understanding the effect of the empty cavity on water dynamics in the carbon nanotube and offering another way to control water properties at the nanoscale.

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Introduction. – The transfer of water molecules through a nanochannel has drawn much attention in recent years [1–5]. Many methods have been proposed to control water transfer properties. A basic but critical process of controlling water transfer is blocking the water nanochannel. So far, many methods have been reported to block a water nanochannel. The first method was reported by Wan *et al.* in 2005 [6]. They investigated water molecules in a carbon nanotube under continuous inward deformation and found that the flux and occupancy are almost kept as a constant within a deformation of 0.2 nm but decrease sharply with another deformation of 0.06 nm. In their studies, the water nanochannel is in the off state when the inward deformation reaches 0.26 nm. The second method was proposed by Li *et al.* in 2007 [7]. They studied water permeation across a nanochannel under the influence of a mobile external charge. They showed an on-off behavior by a mobile $1.0 e$ when the distance is less than a critical distance of 0.085 nm. The third way of blocking a water nanochannel was achieved by adding the dipolar molecules [8]. The four half rings of dipolar molecules outside the nanochannel result in the on-off behavior of water molecules in the nanochannel. Recently, Liu found that cations block the water flow through a narrow carbon

nanotube because of the interactions between cations and aromatic rings [9].

As we know, the transfer properties of water molecules through a nanochannel are dependent on the structure of the nanochannel. For example, the outside structure affects water transport through the nanochannel greatly [10]. The cone-shaped structure enhances water self-diffusion in the nanochannel [11]. Non-straight nanotubes with bending angle can increase the bidirectional water transfer rate [12,13]. Water channel defects have an important role in affecting water adsorption or transfer states [14–16]. Water molecules also display the new transport behavior in the disjoint nanochannel [5,17–19]. It is reported that the nanojunction or the hourglass shape influence water transfer properties as well [20–22].

Herein, the structure of the nanochannel plays a critical role in tuning water dynamics in the nanochannel. Much attention is paid to the inward deformation or the change of the pore entrance. So far, the nanochannel with an empty cavity has been little discussed. We notice that a stable cavity can be formed by means of placing two crossed single-walled carbon nanotubes [23]. And the crossing single-walled carbon nanotube can be joined by electron beam welding to form the empty cavity [24]. Various stable cavities are created and adopted in the experiments and the computer simulations [25–27]. The cavity

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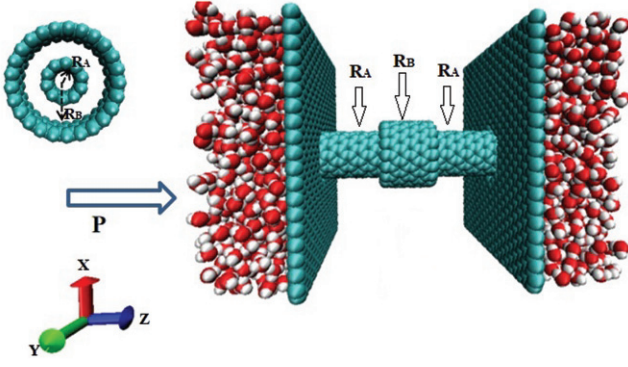


Fig. 1: A snapshot of the simulation system: the red balls represent the oxygen atoms, the white balls are the hydrogen atoms, while the cyan atoms represent the carbon atoms. The inserted figure is the structure of the combined carbon nanotube with an empty cavity: the smaller radius is marked as R_A and the larger radius is marked as R_B . The effective external pressure is applied along the positive direction of z -axis.

plays important roles in influencing the atomic configurations [28]. However, the dynamic properties of water molecules in the various cavities are far from being understood. One important reason is that the cavity is fixed and the size of the cavity has not been considered as a key factor. Another reason is that the cross-section of the cavity is not large enough compared with a complete nanochannel. As a result, many unexpected properties of water molecules in the nanochannel with an empty cavity have not been discovered. Aiming at finding the different properties of water molecules in a nanochannel with a complex structure, we take the cavity size into consideration.

Methods. – The simulation framework is displayed in fig. 1. It contains two graphene sheets with a distance of 4.0 nm, a combined carbon nanotube with an empty cavity and 1875 water molecules. In order to construct the combined carbon nanotube with an empty cavity, we choose two kinds of carbon nanotubes: two (10, 0) carbon nanotubes with a radius of 0.386 nm (marked as R_A) and one carbon nanotube with a large radius (marked as R_B). R_B ranges from 0.386 nm to 1.119 nm. The combined carbon nanotube is a complete (10, 0) carbon nanotube when R_B is 0.386 nm. The length of the empty cavity is 1.0 nm. The TiP3P water model is adopted in the simulations [29] and the carbon atoms are treated as the uncharged Lennard-Jones particles with a cross-section of $\sigma_{CC} = 0.34$ nm, $\sigma_{CO} = 0.3275$ nm, and a depth of the potential well of $\varepsilon_{CC} = 0.3612$ kJ \cdot mol $^{-1}$, $\varepsilon_{CO} = 0.4802$ kJ \cdot mol $^{-1}$ [30]. In order to achieve a unidirectional movement of the water molecules in the nanochannel, we adopt the method used in the published article and apply an external force to all the water molecules with an acceleration of 0.1 nm \cdot ps $^{-2}$ [6,7]. The external pressure of the water molecules in bulk is related to the position and the effective pressure between the two ends of the combined carbon nanotube is about 397 MPa according to the

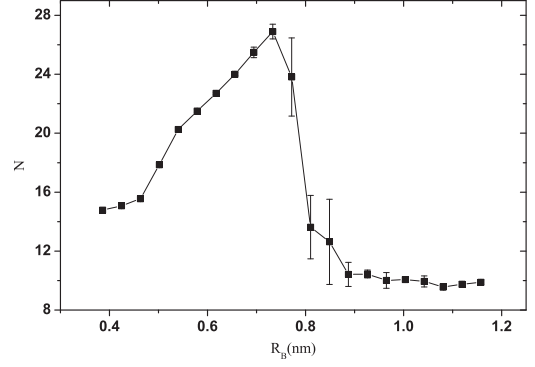


Fig. 2: The average number of water molecules, N , in the combined carbon nanotube as a function of R_B .

pressure used in the simulations [6]. The combined carbon nanotube is empty without water molecules with the purpose of observing the diffusion properties in the combined carbon nanotube with a cavity initially.

Molecular dynamics simulations with GROMACS 4.0.5 are performed [31], and the temperature is maintained at 300 K with the thermostat of Nosé and Hoover [32,33] with a time constant of 0.5 ps. All simulations are carried out under the NVT ensemble. Periodic boundary conditions are applied to all three directions. The total simulation time is 55 ns with a time step of 2 fs. Water flow reaches a steady state after a small transient time of less than 0.2 ns [18]. Therefore, we discard the data produced in the first 5 ns of the simulation. The remaining 50 ns are used to calculate the water properties in the combined carbon nanotube. 1.4 nm is chosen as the cut-off distance for the Lennard-Jones interaction.

Results and discussion. – The adsorption of water molecules in the combined carbon nanotube is displayed in fig. 2. Increase of R_B will result in the increase of the total volume of the combined carbon nanotube with a cavity. The number of water adsorption in the combined carbon nanotube should increase with increasing R_B :

$$N = \sum_{t=0}^{t=50} \frac{N_a(t)}{n}. \quad (1)$$

We calculate the average number of water molecules in the combined carbon nanotube according to eq. (1), where $N_a(t)$ is the number of water molecules in the combined carbon nanotube at time t , n is the total frames during 50 ns. The simulation result is contrary to our common sense. The average number of water molecules, N , in the combined carbon nanotube can be divided into three different processes when R_B changes from 0.386 nm to 1.119 nm. In the first process, N increases with increasing R_B when R_B changes from 0.386 nm to 0.733 nm. For example, the average number of water molecules in the combined carbon nanotube is 14.7805 when R_B is 0.386 nm. The average number of water molecules in the combined carbon nanotube increases to 26.8968 water molecules

when R_B is set to 0.733 nm. The average number of water molecules in the combined carbon nanotube is in accordance with our expectation in the first stage. However, the average number of water molecules in the combined carbon nanotube does not increase continuously with increasing R_B . The average number of water molecules in the combined carbon nanotube decreases sharply when R_B changes from 0.733 nm to 0.849 nm. The number of water molecules in the combined carbon nanotube decreases to 12.6297 water molecules when R_B increases to 0.849 nm. Although the volume of the combined carbon nanotube still increases with increasing R_B from 0.733 nm to 0.849 nm, the average number of water molecules has a sharp reduction in the second stage. The result is out of our expectation. The increasing volume of the combined carbon nanotube cannot hold more water molecules in its interior space in the second stage. Lastly, the average number of water molecules in the combined carbon nanotube is almost kept as a constant when R_B changes from 0.849 nm to 1.119 nm. The number of water molecules has seldom been affected by the change of R_B in the third stage. The adsorption behavior of water molecules is almost unchanged if the macroscale cavity increases by a few nanometers. However, the adsorption behavior of water molecules in the combined carbon nanotube changes obviously when the cavity increases by a few nanometers. To our knowledge, it is the first time to tune the adsorption of water molecule in the combined carbon nanotube by the size of the cavity.

From fig. 2, we can say that the adsorption of water molecules in the combined carbon nanotube can be tuned by the magnitude of R_B , and water adsorption experiences three different processes with increasing R_B . One may concern the transfer properties of water molecules through the combined carbon nanotube under the influence of R_B . We show the average transfer rate, V_f , through the combined carbon nanotube as a function of R_B on the basis of eq. (2) in fig. 3:

$$V_f = \frac{N_f(t = 50)}{50}. \quad (2)$$

$N_f(t = 50)$ is the total number of water molecules transferred from the left end of the combined carbon nanotube to the right end of the combined carbon nanotube during 50 ns. The tendency of V_f decreases with increasing the magnitude of R_B under the external pressure difference. The tendency of V_f can also be divided into three stages. V_f decreases slightly when R_B changes from 0.386 nm to 0.733 nm in the first stage. For example, the transfer rate of water molecules through the combined carbon nanotube is 26.36 water molecules per nanosecond when R_B is 0.386 nm. The transfer rate of water molecules decreases to 22.94 water molecules per nanosecond when R_B increases to 0.733 nm. The water transfer rate through the combined carbon nanotube is maintained at a fast transfer rate in the first stage. However, the tendency of V_f has an obvious decrease when R_B changes from

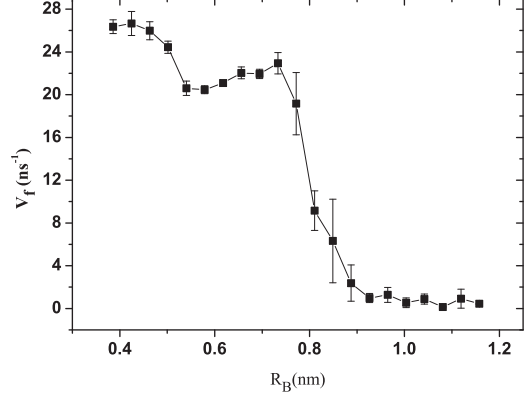


Fig. 3: The average transfer rate of water molecules, V_f , through the combined carbon nanotube as a function of R_B .

0.733 nm to 0.849 nm. The transfer rate of water molecules through the combined carbon nanotube reduces to 6.32 water molecules per nanosecond. It is to say, V_f has a sharp reduction in the second stage. The transfer rate of water molecules changes from a fast water transfer rate to a slow water transfer rate in the second stage. In the third stage, the water transfer rate is maintained at a very slow level when R_B changes from 0.849 nm to 1.119 nm. Compared with the water transfer rate in the first stage, the combined carbon nanotube in the third stage can be treated as in the blocked state. So far as we know, blocking the water nanochannel has been achieved by pressing the inward displacement, adding single-point charges or dipolar molecules. However, a different blocking mechanism of the water nanochannel can be achieved by a large empty cavity. There is one important and critical size of R_B . The critical size of R_B is 0.733 nm. Water transfer through the combined carbon nanotube is not affected obviously by the empty cavity when R_B is below 0.733 nm. However, the water transfer through the combined carbon nanotube is significantly influenced by the size of R_B when R_B is above 0.733 nm.

According to fig. 2 and fig. 3, we can say that both the adsorption and transfer properties of the water molecules can be tuned by the parameter R_B . In order to dig out the blocking mechanism, we pay attention to the interaction between water molecules and the carbon framework. As the Lennard-Jones interaction plays crucial roles in affecting water properties, we calculate the Lennard-Jones interaction between water molecules and the combined carbon nanotube on the basis of eq. (3) and display the result in fig. 4(a):

$$V_{LJ} = 4\epsilon_{CO} \left[\left(\frac{\sigma_{CO}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{CO}}{r_{ij}} \right)^6 \right]. \quad (3)$$

ϵ_{CO} and σ_{CO} are the Lennard-Jones potential parameters, r_{ij} is the separation between the water molecules and the carbon atoms. Since the middle part of the combined carbon nanotube structure changes with increasing

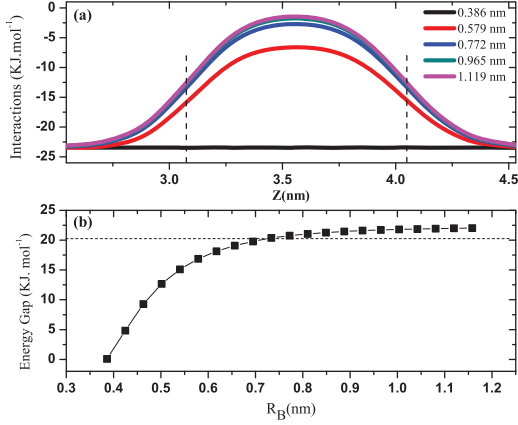


Fig. 4: (a) The Lennard-Jones interaction between water molecules and the combined carbon nanotube as a function of position when R_B is 0.386 nm, 0.579 nm, 0.772 nm, 0.965 nm and 1.119 nm. The dashed line represents the position of the empty cavity. (b) The energy gap as a function of R_B . The dotted line represents the hydrogen bond energy.

R_B , we especially display the Lennard-Jones potential between water the molecules and the combined carbon nanotube near the cavity. In order to display the tendency of the Lennard-Jones potential between water the molecules and the combined carbon nanotube, we just show the interaction when R_B equals 0.386 nm, 0.579 nm, 0.772 nm, 0.965 nm and 1.119 nm, respectively. It is obvious that the Lennard-Jones interaction between water molecules and the carbon framework is dependent on the value of R_B . The Lennard-Jones interaction between water molecules and the carbon framework has a slight difference and is almost kept as a constant line when R_B is 0.386 nm. However, there is a peak when R_B equals 0.579 nm, 0.772 nm, 0.965 nm and 1.119 nm. Compared with the case of 0.386 nm, the Leannard-Jones interaction between water molecules and the carbon framework has a peak. With increasing R_B , the value of the peak point increases. If we define the energy gap as the Lennard-Jones interaction difference between the maximum value of the Lennard-Jones interaction ($0.386 \leq R_B \leq 1.119$) and the minimum value of the Lennard-Jones interaction ($R_B = 0.386$). The energy gap is shown in fig. 4(b). The energy gap is almost zero in the middle part of the combined carbon nanotube when R_B is 0.386 nm. The nanochannel will not hinder the transfer of water molecules through the combined carbon nanotube with $R_B = 0.386$ nm. The energy gap for water molecules is getting larger and larger with increasing R_B . That is why the trend of V_f decreases with increasing R_B . The hydrogen bond is important for the formation of water chains. A very accurate energy of water/water hydrogen bond is $-4.84 \text{ kcal} \cdot \text{mol}^{-1}$ ($-20.25 \text{ kJ} \cdot \text{mol}^{-1}$) [34]. The energy gap reaches the hydrogen bond energy (the dotted line in fig. 4(b)) when R_B equals 0.733 nm. The structure of water molecules in the nanochannel may be different due to the competition between the energy gap and the

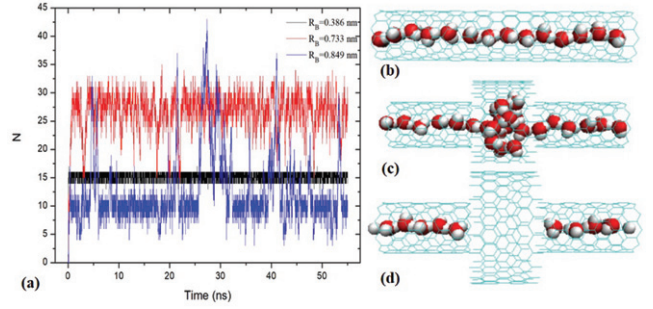


Fig. 5: (a) The number of water molecules, N , in the combined carbon nanotube as a function of time. (b) The snapshot of water molecules in the combined carbon nanotube when R_B is 0.386 nm. (c) The snapshot of water molecules in the combined carbon nanotube when R_B is 0.733 nm. (d) The snapshot of water molecules in the combined carbon nanotube when R_B is 0.849 nm.

hydrogen bond energy. The water molecules form water chains when the energy gap is weaker than the hydrogen bond energy. However, the water structure changes if the energy gap is stronger than the hydrogen bond energy.

In order to test our conjecture, we display the number of water molecules in the combined carbon nanotube as a function of time and show three snapshots in fig. 5. We choose three typical points when R_B equals 0.386 nm, 0.733 nm and 0.849 nm. Figure 5(a) displays the number of water molecules in the combined carbon nanotube as a function of time. Water molecules fill the empty combined carbon nanotube with $R_B = 0.386$ nm and the water number fluctuates slightly during the simulations. The number of water molecules increases when R_B increases to 0.733 nm. The combined carbon nanotube with $R_B = 0.733$ nm can be full filled with water molecules. However, most of the simulation time, the number of water molecules in the combined carbon nanotube with $R_B = 0.849$ nm maintains a small number, and the combined carbon nanotube cannot be fully filled with the stable water chains. Figure 5(b) displays water molecules in the combined carbon nanotube when R_B is 0.386 nm. Since the energy gap is almost zero, water molecules form a single file in the nanochannel when R_B is 0.386 nm. Although the energy gap is getting larger, the energy gap is weaker than the hydrogen bond energy when $R_B \leq 0.733$ nm and the water molecules in the combined carbon nanotube can overcome the energy gap and move into the cavity when $R_B \leq 0.733$ nm. We observe water chains in the cavity when $R_B = 0.733$ nm (shown in fig. 5(c)). That is why the number of water molecules in the combined carbon nanotube increases when R_B changes from 0.386 nm to 0.733 nm. However, if the energy gap is stronger than the hydrogen bond energy, the water chains begin to break in the large cavity. As fig. 5(d) shows, water molecules do not form stable water chains and disappear in the cavity when R_B equals 0.849 nm. That is the reason why water molecules decrease sharply

when R_B changes from 0.733 nm to 0.849 nm. Since water chains have been broken when R_B equals 0.849 nm, water molecules still do not form stable water chains in the large cavity when R_B changes from 0.849 nm to 1.119 nm. So water molecules are almost kept as a constant when R_B changes from 0.849 nm to 1.119 nm. The transfer properties of water molecules through the nanochannel can also be explained. Water molecules still form water chains in the cavity when $R_B \leq 0.733$ nm, and result in the fact that the water transfer rate has not been sharply affected in the first stage. However, water chains begin to break when $R_B > 0.733$ nm, water transport properties have been influenced by the cavity obviously.

In this article, we investigate the effect of an empty cavity on water occupancy and water transfer properties. With the increase of the size of the empty cavity, water occupancy increases when the radius of the cavity is below 0.733 nm but it decreases when the radius of the cavity is above 0.733 nm. The transfer rate through the combined carbon nanotube decreases sharply when the radius of the cavity is above 0.733 nm. We confirm that the radius of the cavity plays important roles in affecting water occupancy and water transfer rate. Compared with the results reported by Wan *et al.* [6], we find a different mechanism of reducing the water transfer rate through a one-dimensional carbon nanotube. According to Wan's results, the occupancy and transfer rate are almost kept as a constant within the inward deformation of 0.2 nm but they decrease sharply with another deformation of 0.06 nm. However, the properties of the occupancy and transfer rate of the water molecules in the carbon nanotube with an empty cavity are different from the properties of the occupancy and transfer rate of the water molecules in the carbon nanotube with inward deformation. In our work, the inward deformation is more powerful in reducing the water transfer properties. Our results indicate another possible way to reduce the water transfer rate through a one-dimensional nanochannel. We believe that the occupancy and the transfer rate are not significantly changed if a macro-sized channel increases by a few nanometers under a constant pressure. However, the occupancy and the transfer rate are significantly changed if part of the one-dimensional nanochannel increases by no more than one nanometer under a constant pressure.

Although there are important discoveries revealed by our studies, there are also limitations. First, the external pressure difference is generated by the method of adding an acceleration to all the water molecules. The effective external pressure is relatively low and can be used to investigate the gating effect [6,7]. We believe that the water transfer properties will be changed if a high pressure difference is added to the simulations system. More water molecules are pushed in the empty cavity under a very strong pressure difference. The blocking effect of the empty cavity on the water molecules transfer through the carbon nanotube will disappear if a strong

external difference is applied. As we know, there is an internal water pressure generated by water collision. That is why water molecules can transfer through the narrow nanochannel bidirectionally without the external pressure. If the thickness of the water reservoirs increases, the internal pressure also increases, which will shift the critical point of affecting water properties. As we see, both the external pressure and the internal pressure affect the water transfer through the combined carbon nanotube with an empty cavity. Our results are applicable to low external pressure and low internal pressure. The effect of the external pressure on the water properties in the combined carbon nanotube with an empty cavity if the external pressure difference increases is still unknown. Second, the combined carbon nanotube with an empty cavity consists of one-dimensional carbon nanotubes and a cavity with a large radius. It is interesting to investigate water properties in a combined carbon nanotube with a cavity if R_A increases. Third, the cavity is placed in the middle of the combined carbon nanotube. Whether the position of the cavity affects the results deserves to be investigated. Fourth, the electric field and the magnetic field can change the water transfer properties. No electric field or magnetic field is applied in the simulation system. We cannot predict the results if an electric field or a magnetic field is added to the simulation system. Overall, there are still many conditions that should be considered. We believe that some limitations can be solved if we 1) add a different external pressure, 2) replace the one-dimensional carbon nanotube, 3) change the position of the cavity, 4) add an electric field or a magnetic field to the simulation system. So far, several methods have been reported to reduce the water transfer rate through a nanochannel. Besides the inward deformation, the point charge [7], the dipolar molecules [8] and the cations [9] can reduce the water transfer rate. We believe that the efficiency of decreasing the water transfer rate will be enhanced if the nanochannel with the inward deformation (or point charge, dipolar molecules, cations) couples with the empty cavity.

Conclusions. – In summary, we investigate water occupancy and water transfer properties in a combined carbon nanotube with an empty cavity under a low external pressure difference. The size of the empty cavity has an important role in affecting water occupancy and transfer properties. There is a critical radius of the empty cavity. The water transfer rate through the combined carbon nanotube begins to decrease sharply when the radius of the cavity is above the critical radius. The adsorption of water molecules in the combined carbon nanotube increases when the radius of the cavity is below the critical radius but it decreases when the cavity is above the critical radius. The competition between the energy gap and hydrogen bond energy plays a critical role in tuning the water behaviors in the combined carbon nanotube. Our results pave the way for understanding the empty cavity on water molecules in the nanochannel under a low

pressure difference and offering another possible way to control water molecules at the nanoscale.

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