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Citation: Chin. Phys. B . 2018, 27(1): 013101. **doi:** 10.1088/1674-1056/27/1/013101

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TOPICAL REVIEW — Soft matter and biological physics

Control water molecules across carbon-based nanochannels*

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(Received 30 August 2017; revised manuscript received 30 October 2017; published online 22 December 2017)

It is important to know the mechanisms of water molecules across carbon-based nanochannels, which is not only beneficial for understanding biological activities but also for designing various smart devices. Here we review the recent progress of research for water transfer across carbon-based nanochannels. In this review, we summarize the recent methods which can affect water molecules across these nanochannels. The methods include exterior factors (i.e., dipolar molecules and gradient electric fields) and interior factors (namely, cone-shaped structures, nonstraight nanochannels, and channel defects). These factors can control water permeation across nanochannels efficiently.

Keywords: carbon nanotube, water molecules, flow enhancement, confinement

PACS: 31.15.at **DOI:** 10.1088/1674-1056/27/1/013101

1. Introduction

Water is the most important material in the biosphere. Almost all biological activities are carried by water molecules. In human cells, water molecules move in and out of cell membranes by water channels.[1] In general, the mechanisms of water permeation across these water channels are poorly understood. Because, the water channels contain complex structures and various chemical elements. Thus, it is difficult to separate generic causative features of water transport from structures and chemical elements. As a result, it is important to develop model systems to determine the functional relevance of key structural features. Computer simulations and experiments suggest that nanotubes can be filled with water molecules.[2–4] Meanwhile, the behaviors of water molecules in a carbon nanotube share some similar phenomena with these in biological water channels, such as single-file arrangement, wave-like density distribution, wet–dry transition, gating and so on.[2,5–9] This makes carbon nanotubes an attractive medium for the study of water transport across nanochannels. Thus, water permeation across carbon nanotubes have been studied computationally and experimentally.[5,10–13] For the narrowest carbon nanotube (if water molecules can move in it), due to pore restriction, water molecules form a single file, which is important for water desalination.

Despite of recent progress, a key issue is how to affect water across a nanochannel efficiently? Present research usually focus on exterior factors such as pressure, charge, force, electric fields, magnetics and so on.[14–16] Such exterior factors which affect water permeation across single-walled carbon nanotubes (SWCNTs) have been studied tremendously. Another method is changing interior factors of nanochannel itself such as pore of the entrance, channel length, and so on.

In this review, we first clarify the recent exterior factor which can affect water permeation across nanochannels, including dipolar molecules (Section 2.1) and gradient electric fields (Section 2.2). Then we introduce some interior factors which also affect water permeation in the nanochannels recently, including cone-shaped structure (Section 3.1), nonstraight nanochannels (Section 3.2), and channel defects (Section 3.3). This review ends with a summary and outlook in Section 4.

2. Exterior factors

2.1. Dipolar molecules

What is the mechanism of controlling biological water channel gating? Wan *et al.* had studied that an on–off gating behavior can be realized by adding an external force on the carbon nanotube.[17] Furthermore, an on–off gating behavior of water nanochannels was also revealed by using a single external charge of value $+1.0\,e$.[8] As inspired by charged residues in a nanochannel protein such as aquaporin, in particular, due to ionization, coions (and thus counterions) are indispensable in membrane protein. We restructured a system, which contains four half-rings LiF dipolar molecules (see

*Project supported by the Fundamental Research Funds for the Central Universities of China (Grant No. 2015QNA48), the Natural Science Foundation of Jiangsu Province, China (Grant No. BK20150173), the Science and Technology Commission of Shanghai Municipality, China (Grant No. 16ZR1445100), and the National Natural Science Foudnation of China (Grant Nos. 11725521 and 11605285).

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Fig. 1).[9] Each LiF was placed along the radical direction of the single-walled carbon nanotube, where the Li atoms were closer than the F atoms. The dipole moment for each LiF was 6.294 D (1 $D \approx 3.336564 \times 10^{-30}$ C·m). The smallest distance between Li atom and the centerline of the single-walled carbon nanotube was defined as R. As LiF molecules were dipolar molecules, which generated ununiform electric fields in the space. By the finite element method,[18] we studied two-dimensional (2D) electrostatic field strength distributions in the simulation system (see Fig. 2). The results showed that the field distribution was quite inhomogeneous inside the SWCNT, and the area close to the LiF molecules had a higher field strength for $R = 0.533$ nm. In contrast, the electric field distribution inside the SWCNT was much more homogeneous and the field strength was relatively low when $R = 1.856$ nm. When the LiF molecules were located close to the SWCNT (say $R = 0.533$ nm), the electric field strength generated by LiF increased inside the SWCNT, thus it attracted water molecules more strongly. As a result, the transport of water molecules was affected by dipolar molecules. By changing R from 0.533 nm to 1.856 nm, we observed on–off state transitions of water molecules across the nanochannel. As Fig. 3 shows, N_f was always zero as $R < 0.944$ nm, which thus corresponded to an off state of the SWCNT. In contrast, as $R > 0.944$ nm, N_f became nonzero, which was related to an on state of the SWCNT. Besides, the dipolar molecules affected the average water orientations and the number of water molecules in the SWCNT. The average orientations of water molecules in the SWCNT had sharp transitions when R increased from 0.533 nm to 1.856 nm. As R increased, the average orientations fluctuated frequently. Meanwhile, as electric fields decreased in the SWCNT interior when R increased, water molecules had less restriction. Thus, the number of water molecules in the SWCNT decreased as R increased.

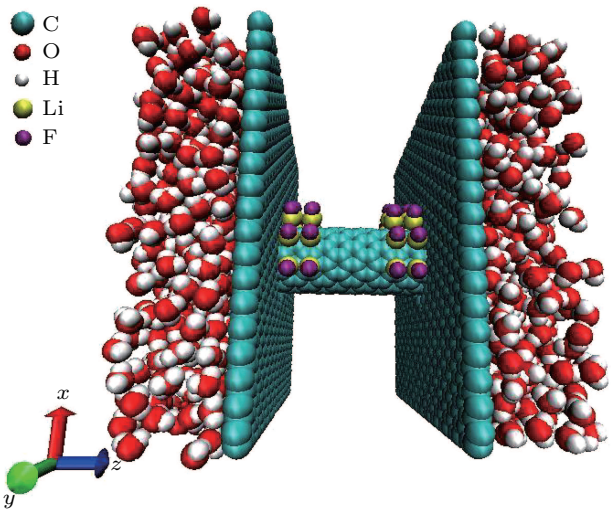


Fig. 1. (color online) Snapshot of the simulation system with a Z-directed SWCNT perpendicularly joining the centers of two graphite sheets. The system is filled by water molecules (H_2O). Four half-rings, each having six lithium fluoride (LiF) dipolar molecules, are symmetrically positioned along radial direction of the SWCNT. Besides atom C, the atoms of H_2O and LiF are shown in different colors. More details, e.g., the positions of the four half-rings, can be found in the main text. For a possible link between this system and a membrane water nanochannel with co-ions and counterions, please refer to Appendix for a qualitative demonstration.[9]

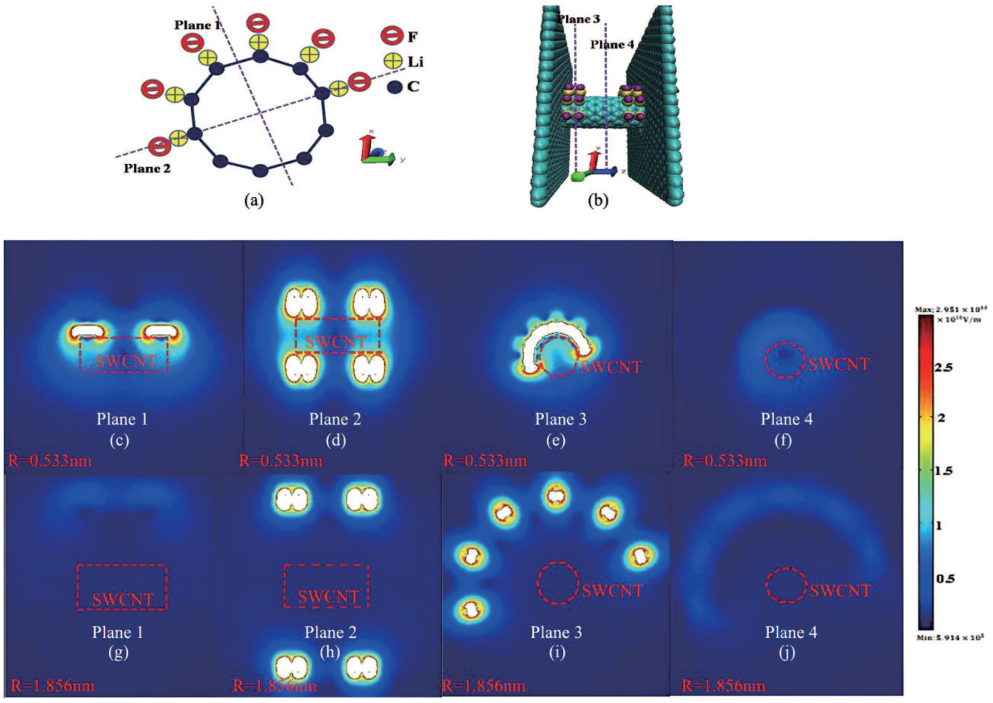


Fig. 2. (color online) Schematic graphs showing four two-dimensional (2D) virtual planes in the simulation system: (a) planes 1 and 2, and (b) planes 3 and 4. The finite element method is performed to show the 2D electrostatic field strength distribution in (c,g) plane 1, (d,h) plane 2, (e,i) plane 3, and (f,j) plane 4, for (c–f), $R = 0.533$ nm and (g–j), $R = 1.856$ nm. In (c–j), the white regions possess the value of the electric field strengths exceeding the bounds of bars. Both the dashed rectangle in (c,d,g,h) and the dashed circle in (e,f,i,j) denote the position of the SWCNT.[9]

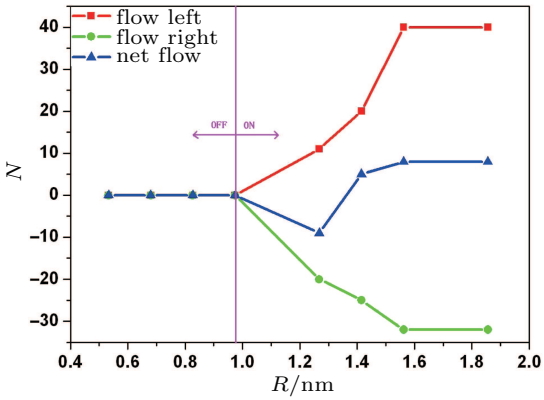


Fig. 3. (color online) Number of water molecules, N_f, flowing across the SWCNT within 20 ns as a function of R.[9]

2.2. Gradient electric field

Achieving a fast, unidirectional flow of single-file water molecules (UFSWM) across nanochannels was important for membrane-based water purification or seawater desalination, where nanochannels located in the membrane should had a diameter small enough so that only water molecules were allowed to enter while other particles larger than a water molecule could not move in. As a result, progress in this direction had been made by designing systems with an osmotic or hydrostatic pressure gradient, with an imbalance of surface tension, with a chemical or thermal gradient, or with external electric fields or charges.[14–16] Despite of recent progress, it is still difficult to control water permeation or to get a fast UFSWM. In order to get a fast UFSWM, we proposed a design for achieving giant pumping of water molecules in a (10, 0) SWCNT with length 2.38 nm in the presence of a linear gradient electric field (GE) field (see Fig. 4).[19] For comparison, we used a uniform electric field (UE). The strengths of UE field and GE field were given by $E = E_a$ and $E = E_a(z/L_z)$, respectively. Here, "+flux" and "−flux" denote the number of water molecules per nanosecond transferring across the SWCNT along the $+z$ and $-z$ axis, respectively. The simulation results were encouraging (see Fig. 5). First, we simulated the system in the absence of electric field, and no obvious net flux was obtained. Second, in the case of the UE fields, for various E_a, all "+flux" and "−flux" occurred, but the net flux maintained a small value ranging from 1.4 to 1.9 water molecules per nanosecond. Third, for the GE fields, "−flux" did not exist, and only "+flux" appeared. The net flux increased as E_a increased significantly. Surprisingly, the maximum speed of the net flux reached 109.2 water molecules per nanosecond at $E_a = 8.0$ V/nm, which was 2 orders of magnitude larger than that of the UE field with $E_a = 8.0$ V/nm. Thus, the GE fields can yield a much more efficient UFSWM across a SWCNT than the UE fields. Why the GE fields can increase UFSWM? Reasons can be found in Fig. 6. We calculated the averaged net electrostatic force, $\langle f_z \rangle$, acting on a water molecule within the SWCNT as a function of E_a in the GE or UE fields. The averaged net electrostatic force $\langle f_z \rangle$ was always nonzero for

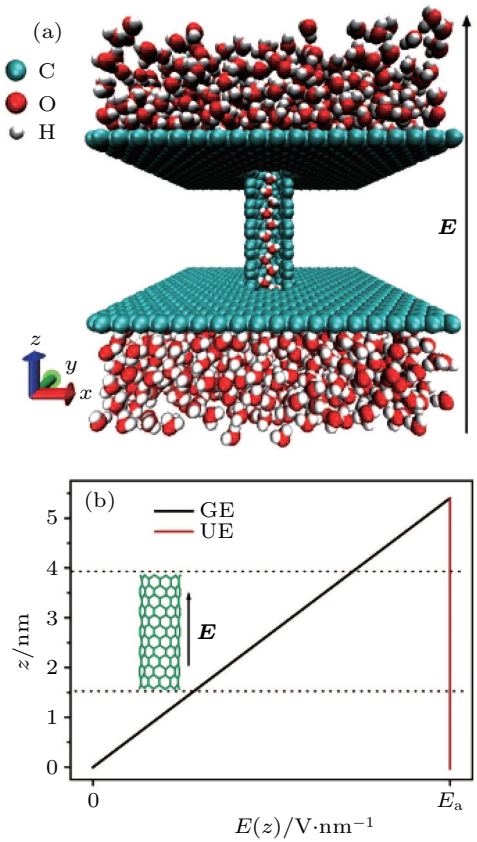


Fig. 4. (color online) (a) Introduction to the simulation box. Two parallel fixed graphite sheets with separation 2.380 nm divide the box (with dimensions $L_X \times L_Y \times L_Z = 4.650\,\text{nm} \times 4.650\,\text{nm} \times 5.434\,\text{nm}$) into three parts. A z-directed, uncapped, semiconducting (10, 0) SWCNT with diameter 0.772 nm and length 2.38 nm perpendicularly joins the two graphite sheets. The box contains 1826 water molecules; within the area between the two graphite sheets, there are no water molecules outside the SWCNT. The bottom of the simulation box is located at $z = 0$, and the two ends of the SWCNT are located at $z = 1.527$ and 3.907 nm, respectively. The box is subjected to a UE or GE field, $\boldsymbol{E}$ directed along the z-axis. (b) The strengths of the UE and GE field are given by $E = E_a$ and $E = E_a(z/L_z)$, respectively. Here $0 < z < L_Z$ and $0 < E_a < 8$ V/nm.[19]

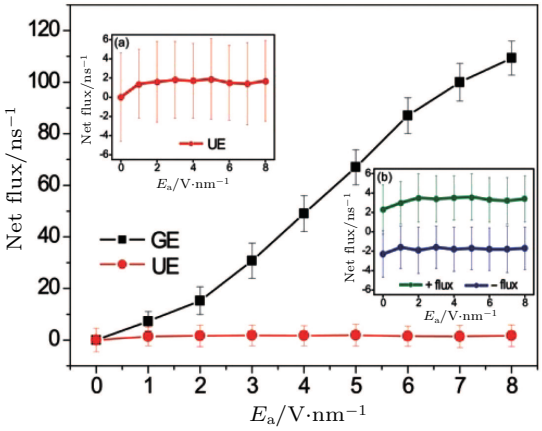


Fig. 5. (color online) Net flux (= "+ flux" − "− flux") of water molecules transporting across the SWCNT in the GE or UE fields. Here, "+ flux" and "− flux" denote the number of water molecules per nanosecond transferring across the SWCNT along the $+z$ and $-z$ axis, respectively. Specifically, "−flux" is always zero for the GE fields. For clarity, inset (a) shows the net flux in the UE field only, which just corresponds to the "+ flux" and "−flux" displayed in inset (b).[19]

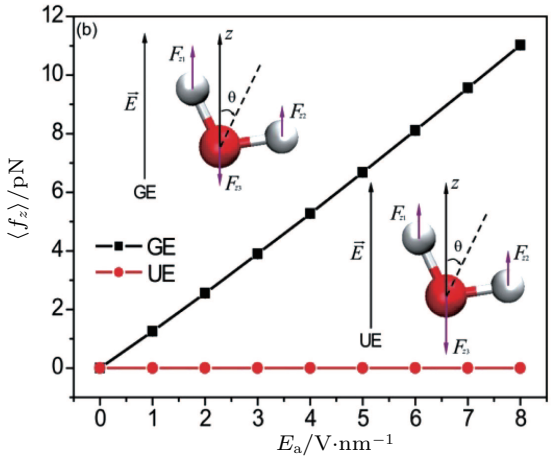


Fig. 6. (color online) The averaged net electrostatic force, $\langle f_z\rangle$, acting on a water molecule within the SWCNT as a function of Ea in the GE or UE fields. Clearly, $\langle f_z\rangle$ is nonzero for the GE fields (with $E_a > 0$ V/nm) and increases as E_a increases. However, $\langle f_z\rangle$ is always zero for the UE fields. This can be understood according to the two insets: (left inset) for a water molecule in the GE field, the electrostatic forces acting on one oxygen atom and two hydrogen atoms always satisfy $f_{z1} + f_{z2} > f_{z3}$, (right inset) for a water molecule in the UE field, the electrostatic forces satisfy $f_{z1} + f_{z2} = f_{z3}$, thus yielding a zero net force, $f_z = f_{z1} + f_{z2} - f_{z3} = 0$.[19]

the GE fields (with $E_a > 0$) due to $f_z = F_{z1} + F_{z2} - F_{z3} > 0$ as shown in the left inset and also increased as E_a increased. In this condition, each water molecule in the presence of the GE field was exerted on a nonzero net force which drove the molecule to move. However, $\langle f_z\rangle$ was always zero in the presence of UE fields, due to $f_z = F_{z1} + F_{z2} - F_{z3} = 0$ as shown in the right inset. That is why the GE electric field can get a fast UFSWM.

3. Interior factors

3.1. Cone-shaped structure

In the membrane, there are various water channels. The structure of the water channel varies differently. However, most simulation works treated nanochannels as straight ones in order to simplify the simulation system. In practice, the shape of the nanochannel plays important roles in selecting water or ions permeation.[20,21] Inspired by the noncylindrical shape of the Escherichia coli glycero and the voltage-sensitive sodium channel,[20,22] we designed a cone-shaped nanochannel as a model noncylindrical nanochannel to investigate the effect of channel structure on the permeation of water molecules.[23] The cone-shaped and the construction process are shown in Fig. 7. In our construction, each end of the cone-shaped SWCNT only allowed a single molecule to enter or exit. Meanwhile, the volume of the con-shaped nanochannel increased as θ increased. Due to the volume increases,

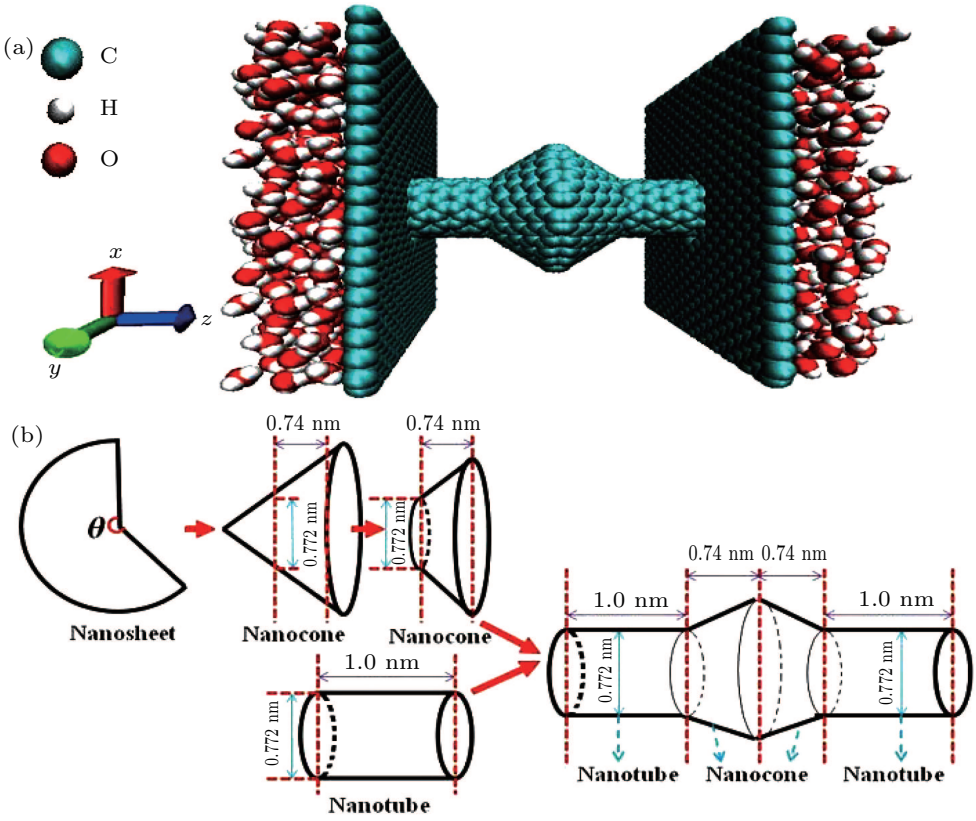


Fig. 7. (color online) (a) A snapshot of the simulation system with one Z-directed nanochannel (namely, a nanotube-nanoconenanotube with the cylindrical-cone-cylindrical shape, which we call "cone-shaped SWCNT" for simplicity) perpendicularly joining the centers of two graphite sheets. Atoms are shown in different colors (or gray scale); (b) the details for constructing the cone-shaped SWCNT. Note the Z-directed length of the nanocone area between the two nanotubes is fixed for all θ's throughout this work. Clearly, a larger angle of a graphite nanosheet, θ, corresponds to a larger volume (interior space) of the nanocone area. Incidently, $\theta = 0°$ stands for the case where the whole SWCNT between the two graphite sheets has a cylindrical shape.[23]

the number of water molecules increased. The average diffusivity of water molecules reflected water mobility in the con-shaped nanochannel. The three components of the average diffusivity along the X, Y, Z axes, D_X, D_Y, and D_Z showed different behaviors with increasing θ (see Fig. 8). Both D_X and D_Y increased as θ increased. The results were easy to understand. As θ increased, the volume of the con-shaped nanochannel increased. So water molecules had less confinement, D_X and D_Y increased as θ increased. However, D_Z displayed different behaviors as increasing θ compared with D_X and D_Y. D_Z increased when $\theta < 120°$, but decreased when $\theta > 120°$. As a result, the average transfer rate of water molecules across the con-shaped, V_f, increased as θ increased. It should be noticed that V_f increased rapidly when $\theta < 120°$; V_f increased slowly when $\theta > 120°$. Figure 9(b) shows the dynamical process of water transfer number as a function of time when θ ranged from 0° to 240°. Figure 9(c) shows the enhancement ratio increased as θ increased. The enhancement ratio increased as θ increased rapidly when $\theta > 120°$; we called this "enhancement behavior". It should be noted that the enhancement ratio tends to be saturated as θ is large enough; we call this "saturation behavior", as the cone-shaped nanochannel restructured by us had one cone-shaped structure. In order to answer whether more nanocone areas will enhance the water flow up to a high value or not. We restructured a system contained more nanocone areas. The simulation results are shown in Fig. 10, which indicates that the permeation ability of water molecules across the cone-shaped SWCNT was enhanced as the nanocone areas number increased.

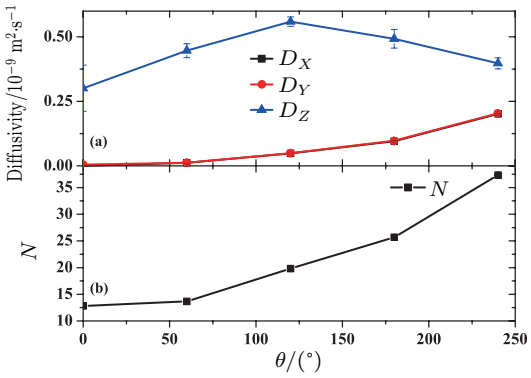


Fig. 8. (color online) (a) Three components D_X, D_Y, and D_Z of the average diffusivity of water molecules within the nanochannel as a function of θ, along the X, Y, and Z axes, respectively. The two curves for D_X and D_Y are overlapped because the nanochannel is symmetrical with respect to the X and Y axes. (b) The average number, N, of water molecules within the cone-shaped SWCNT as a function of θ. The solid lines in both (a) and (b) are a guide to the eye. Error bars are included in both (a) and (b); the error bar is smaller than the symbol point for both D_X and D_Y in (a) and for N in (b).[23]

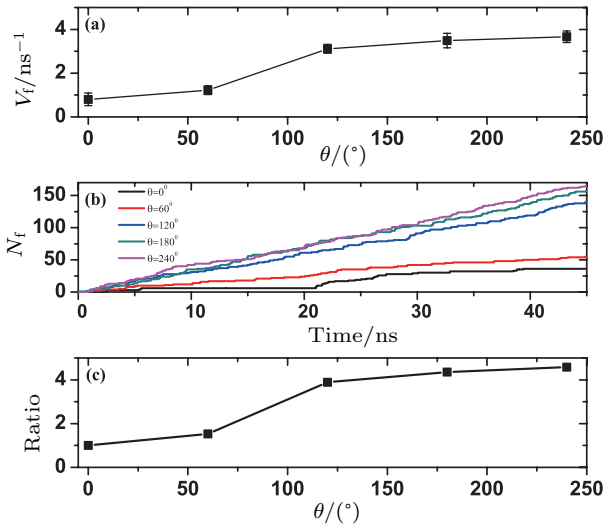


Fig. 9. (color online) (a) The average rate of transfer of water molecules, V_F, flowing across the cone-shaped SWCNT as a function of θ. Error bars are included. (b) The number of water molecules, N_f, flowing across the cone-shaped SWCNT as a function of time when θ varies from 0° to 240°. (c) Enhancement ratio versus θ. Here, the enhancement ratio is just the ratio between N_f of each θ and that of $\theta = 0°$ at time 45 ns as displayed in (b). The curves in (a) and (c) are a guide to the eye.[23]

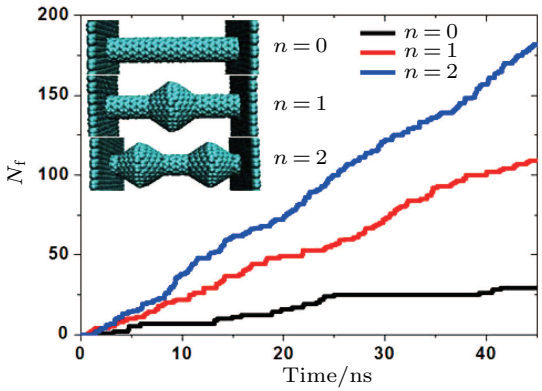


Fig. 10. (color online) The number of water molecules, N_f, flowing across the cone-shaped SWCNT as a function of time, for different numbers of nanocone areas, n.[23]

3.2. Nonstraight nanochannels

As the structure of water channel varies differently, nonstraight nanochannels are indispensable as well.[24] For example, Murata *et al.* reported that biological water nanochannels are generally nonstraight as a result of natural selection.[25] Various nanostructures of carbon nanotubes are reported, such as L-junction, Y-junction, T-junction, and so on.[26,27] Whether a bending nanochannel had an effect on water permeation? In order to solve this problem, we designed a nonstraight according to Han's experimental observation[24] (see Fig. 11). The SWCNT designed by us had a bending angle of φ in its center portion, and two straight (10,0) SWCNTs were connected by appropriately adding extra carbon rings shaped with triangle, quadrilateral, and pentagon in the position of the junction. We prepared 13 systems with bending angles from 35° to 180°.[28] The case of 180° represents the case of a straight SWCNT. All the SWCNTs with different φ weer set to possess the same central path, $\lambda = 3.8$ nm. If the rate of

transfer here was defined as the sum of the numbers of water molecules, which had passed through the whole SWCNT from one mouth to another, per nanosecond. By molecular dynamics simulations, we found that for the nanotube with $\varphi = 35°$, the maximum bending angle in this work, the result of rate of transform was 9.1 ns^{-1}. However, the result of the straight nanotube with $\varphi = 180°$ is 2.6 ns^{-1}. The enhancement ratio between the two tubes in their work can reach up to 3.5. We found that the transfer rate of water molecules across the bending nanochannel increased with the decay of φ (see Fig. 12). The process of enhancement properties of water molecules across the bending nanochannel experienced two different processes. As φ decreased from 60° to 35°, the number of the rate of transfer raised remarkably. However, when φ varied from 180° to 60°, the rate of transfer did not change significantly, but only slightly increased according to the overall trend. These results indicated that water molecules inside a sightly distorted (i.e., $\varphi > 60°$) cannot guarantee a high enhancement ratio. Why a bending nanochannel can increase water molecules transfer flow rate? By calculating the profiles of the potential of mean force along the Z-axis (see Fig. 13), we gave a reasonable analysis. In the case of straight nanotube with $\varphi = 180°$ and slightly bending nanotube with $\varphi = 120°$, the free energy barriers were higher and almost flat. However, for the heavily bending nanotubes with $\varphi = 35°$ and 60°, there exited appreciable shaking in the center of part free energy barrier which were still lower than that of the straight case and slightly bending tube. Thus, water molecules had to surmount the potential barriers, which were lower in smaller bending angle nanotubes, to go through the nanotube from one mouth to another. In this way, the lower free energy barrier from the stronger interaction among water improved the transfer rate when water molecules go through the heavily bending carbon nanotubes with small φ.

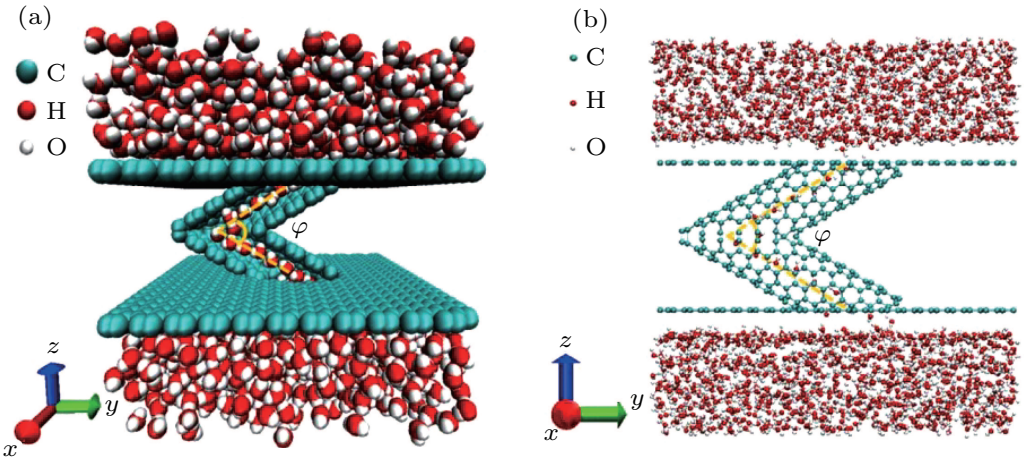


Fig. 11. (color online) (a) A perspective view of the simulation system with a nonstraight SWCNT embedded between two parallel graphite sheets. The bent corner in the SWCNT is denoted by an angle of φ. We show the inner part of the SWCNT by removing some carbon atoms; the orange dashed line indicates the central path across the SWCNT, whose length is λ. (b) An orthographic projection of the model SWCNT with $\varphi = 60°$.[28]

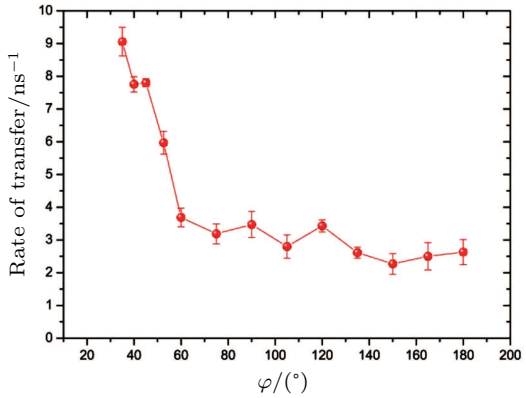


Fig. 12. (color online) Rate of transfer of water molecules through SWCNTs with different $\varphi = 35°$, 40°, 45°, 52.5°, 60°, 75°, 90°, 105°, 120°, 135°, 150°, 165°, and 180°. Here $\varphi = 180°$ denotes the straight SWCNT. The line is a guide for the eye; each symbol is accompanied by an error bar. Here we have divided the data of each system from 15 to 85 ns by seven intervals and calculated the means of the rate of transfer for the seven groups of data to get the error bars. Parameter: $\lambda = 3.8$ nm.[28]

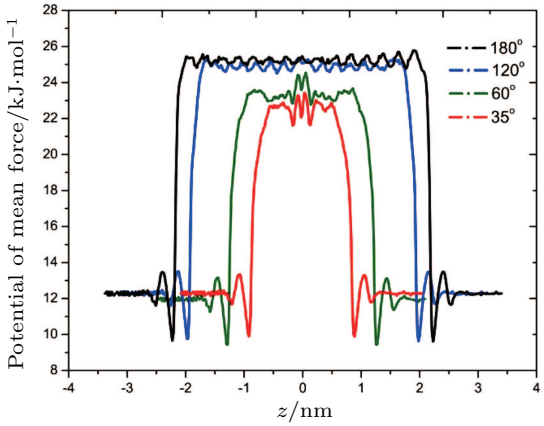


Fig. 13. (color online) Potential of mean force (PMF) profiles along the Z-axis in systems with nanotubes bendng angle $\varphi = 35°$, 60°, 120°, and 180°, and the potential of mean force was calculated by $-K_B T \ln[P(N)]$, where P is the average probability of water molecules along the Z direction, K_B is the Boltzmann constant, and T is the temperature.[28]

3.3. Channel defects

Controlling water molecules through a nanochannel by an electric field is more convenient. Thus, many methods are proposed to control water molecules through the nanochannel by the electric field.[7,19] In practice, single-walled carbon nanotube defects are usually indispensable. Such defects were shown to greatly affect transport individual nanotubes[29] as well as the electronic and mechanical properties of carbon nanotubes.[30–32] The defects can also greatly influence the localization of magnetic and electronic excitation in graphene nanotubes[33] and water molecules through a nanochannel.[34] Besides, the electric field greatly influences the surface properties of graphene-like materials.[35] However, how the SWCNTs with defects affect water permeation under an electric field has rarely been discussed. It is widely accepted that the external conditions of the nanochannel system greatly affects the permeation of water molecules. Many external conditions (say, adding external mechanical forces, pressure gradient, or electric fields/charges) are applied in these fields for studying the transport of water molecules through nanochannels, while taking the nanochannel without defects.[36–43] In order to investigate the effect of defects on water permeation under the electric fields, we designed a defective single-walled carbon nanotube (DSWCNT) as a model of a defective nanochannel (see Fig. 14).[44] In our system, there were six defects in the nanochannel, every defect was designed by removing six carbon atoms (a circle of carbon atoms), a uniform electric field was applied along Y-direction, which was perpendicular to the DSWCNT. Whether the defects had an effect on water molecules under the uniform electric fields? For comparison, we gave the number of water molecules, N_a, in the DSWCNT or perfect single-walled carbon nanotube (PSWCNT) as a function of time under the same electric field, 1.0 V/nm (see Fig. 15). Initially, the DSWCNT (or the PSWCNT) was full of water molecules. We found that the responses of water molecules in the DSWCNT were faster than the responses of water molecules in the PSWCNT. The number of water molecules in the PSWCNT fluctuated with small fluctuations. However, the number of water molecules in the DSWCNT decreased rapidly under 1.0 V/nm. It just took no more than 0.2 ns to achieve a fast wet–dry transition. Thus, DSWCNT was much energy-saving structure compared with PSWCNT. Now, a question was purposed, how strong electric field must be added to control a fast wet–dry transition. By molecular dynamics simulations, we found that there was a critical point of electric field, $E_c = 0.32$ V·nm (see Fig. 16). The transfer rate of water molecules through the DSWCNT had not been affected dramatically by the electric field, and N_f maintained a fast and stable transfer rate. However, N_f decreased to nearly zero if the electric field above the critical electric field. The average number of water molecules in the DSWCNT, N_a shared a similar phenomena below or above the critical electric field. What happened on the critical electric field? We displayed dynamic process of a wet–dry phase transition in Fig. 16(c). Initially, the DSWCNT was full of water molecules. The number of water molecules in the DSWCNT reduced a lot and the DSWCNT was partially dry when time was 3 ns. When time was 6 ns, the DSWCNT was almost completely dry and almost no water molecules existed in the DSWCNT. A nanochannel may exist many defects. More defects in a DSWCNT enhanced or decreased the wet–dry phase transition? We attempted to change the number of defects from six to one, and found that the critical electric field was affected by the number of defects. The tendency of critical electric field showed that E_c was reduced if the number of the defects increased (see Fig. 17). It meant that it was easier to achieve a wet–dry phase transition if the DSWCNT with more defects.

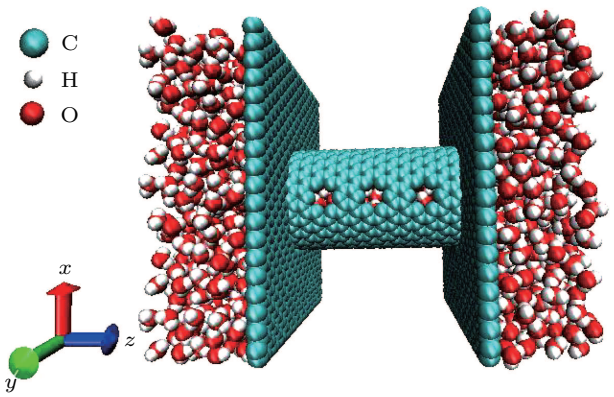


Fig. 14. (color online) Snapshot of the simulation system with a Z-directed DSWCNT perpendicularly joining the centers of two graphite sheets. The system is filled by water molecules (H_2O). An uniform electric field is applied along Y-direction, which is perpendicular to the DSWCNT. There are six defects on the DSWCNT. The defects distribute symmetrically.[44]

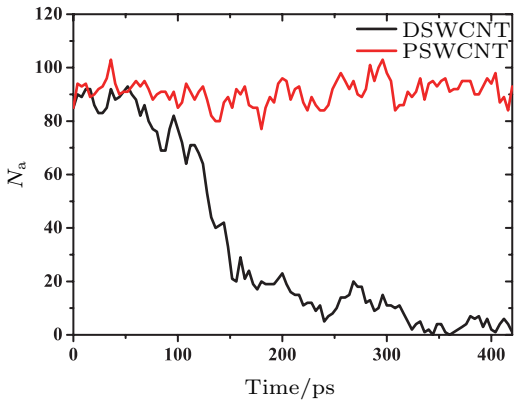


Fig. 15. (color online) The number of water molecules, N_a, in a DSWCNT shown in black (or a PSWCNT shown in red) as a function of time (with step size 2 fs) under the electric field strength 1 V/nm.[44]

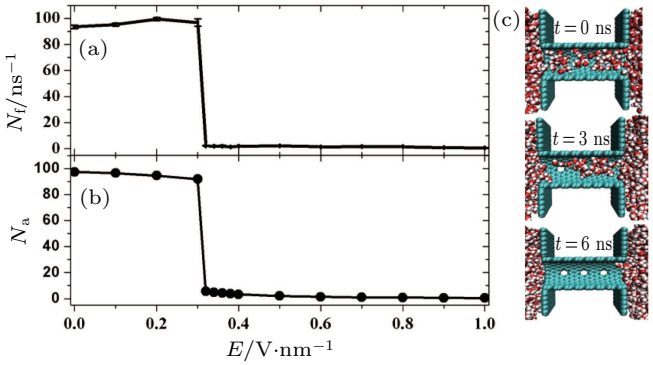


Fig. 16. (color online) (a) The number of water molecules flowing across the DSWCNT, N_f, as a function of the electric field. (b) The number of water molecules in the DSWCNT, N_a, as a function of the electric field. (c) A dynamic wet–dry phase transition under the critical electric field 0.32 V/nm.[44]

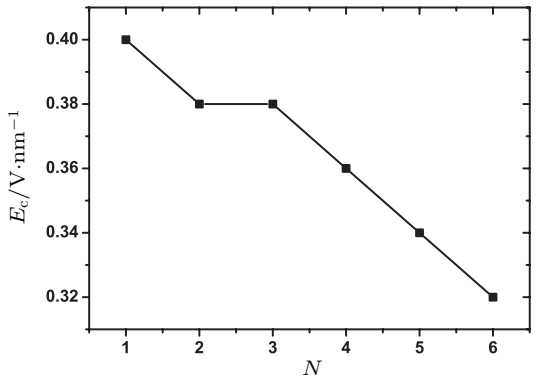


Fig. 17. The critical electric field, E_c, as function of the number of defects, N.[44]

4. Summary and outlook

The transfer of water molecules across carbon-based nanochannel has plenty of applications and meanings. Methods of controlling water transfer ability across nanochannels are mainly due to exterior or interior factors. This review shows recent progress on water transfer cross a carbon-based nanochannel. For example, LiF dipolar molecules could achieve on–off transitions, GE fields could drive water molecules across a nanochannel more efficiently when compared with UE fields, the transfer rate of water molecules increased with either increasing volume of a cone-shaped structure or decreasing bending angle, and more nanochannel defects will decrease the critical electric field of the wet–dry phase transitions. These recent progresses are beneficial for controlling water permeation processes. Despite of the recent progress, numbers of questions might need to be investigated systematically.

(i) It is necessary to investigate interior factors coupling with exterior factors. For example, what will happen if the cone-shaped structure or nonstraight nanochannels adding pressure differences? Is it still increasing or decreasing water transfer ability by changing the volume of cone-shaped structure or the bending angle? Whether does the on–off transition point shift for dipolar-molecule-controlling water permeation if the system contains pressure differences.

(ii) It is necessary to explain the simulation results clearly. In most existing simulation works, authors explained their results according to the trajectories of molecules during the simulation processes. However, this is not convincing all the time. It would be better to explain the simulation results according to the true physics.

(iii) There are other interior and/or exterior factors which can affect water transfer across carbon-based nanochannels. These factors should be searched and investigated.

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