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Water Transport with a Carbon Nanotube Pump

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ABSTRACT Transportation of water molecules in a carbon nanotube based on an energy pump concept is investigated by molecular dynamics simulations. A small portion of the initially twisted wall of a carbon nanotube is employed to function as an energy pump for possible smooth transportation of water molecules. The momentum and resultant force on a water molecule and the corresponding displacement and velocity of the molecule are particularly studied to disclose the transportation process. The efficiency of the transportation is found to be dependent on the size of the energy pump. Once the process for the transportation of one molecule is elucidated, transportations of 20 water molecules are simulated to investigate the effect of the environmental temperature and fluctuations in the nanotube channel on the transportation. It is revealed that the accelerated period of multiple water molecules is longer than that in the transportation of a single water molecule. In addition, the fluctuations in the nanotube wall due to the buckling propagation and a higher environmental temperature will all lead to obvious decreases in the water velocity and hence retard the transportation process.

KEYWORDS: water transportation · carbon nanotubes · van der Waals energy · energy pump · molecular dynamics simulations

The remarkable electrical, mechanical, and thermal properties[1−3] of carbon nanotubes (CNTs) enable them to be used for the development of devices for microelectromechanical and nanoelectromechanical system applications. The possible employment of CNTs in transporting atoms and molecules, owing to their large surface area and smooth wall, would have a wide range of applications, such as spot-welding, novel biomedical therapies,[4,5] and nanopumping devices for atomic transportation.[6]

The migration of carbon interstitials in CNTs under electron irradiation was observed.[7] Subsequently, an experiment revealed high mobility of carbon atoms inside CNTs and demonstrated their potential as a pipeline for the transport of carbon atoms.[8] A nanopipette action for metals using multiwalled CNTs was demonstrated experimentally.[9] The electromigration forces, created at high electron current densities, were found to enable the transport of material inside the hollow core of the CNT. Since CNTs have been found to be manipulated by facilities, such as the tip of an atomic force microscope, effective applications of the deformed CNTs could have potential on atomic transportation. Elastic torsional response and compression of CNTs encapsulating molecules and atoms have even been investigated to study the change of mechanical properties of CNTs.[10] The transportation of helium atoms in a single-walled CNT subjected to torsion was reported,[11] and the efficiency of the atomic transportation was found to be dependent on the torsion loading rate as well as the temperature in the process. Simulations showed that the transportation is a result of kink propagation initiated in the twisted nanotube through the van der Waals force between the nanotube and the helium atoms. In experiments, application of a torsion motion to a CNT was found to be practicable. A twist of a single-walled CNT as high as 180° has been realized experimentally in a design of a pendulum system with resonant frequency on the order of megahertz.[12] The device consists of a metal block suspended on an individual single-walled CNT. The CNT can be twisted by applying electrostatic torque on the metal block using an external electrical field.

Microflow in microcapillaries has great potential in the areas of nanorobotices, helium energetics, medical drug delivery, micropumps, microarays, atom optics, chemical process control, and molecular medicine.[13,14] Water transportation in CNTs has been investigated widely to explore the potential of CNTs as microcapillaries. It was shown that in long CNTs, when the orientation of the water molecules is maintained along one direction, a net water transport along that direction can be at-

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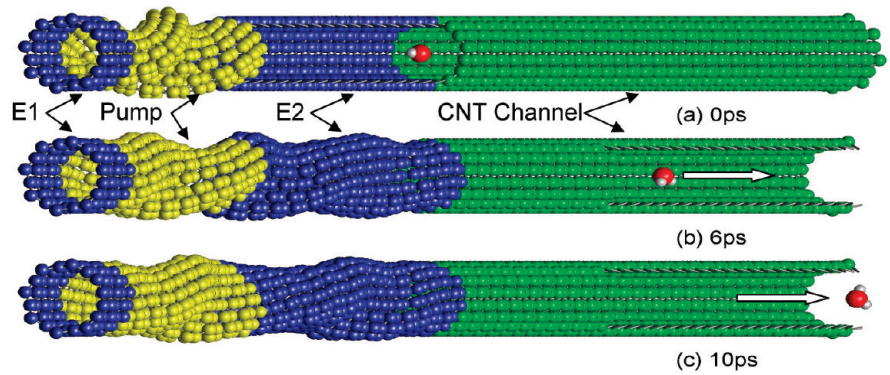

Figure 1. Introduction of an energy pump for transportation of one water molecule in a zigzag (8,0) CNT channel. E1 (blue) and E2 (blue) are fixed, and a pre-twisted angle, 135°, is applied to E1, which results in a torsion buckling of the pump (yellow) as shown in (a) snapshot at 0 ps. Once the restraint on E2 is removed, the potential energy stored in the pump will push the water molecule traveling along the CNT channel (green). The water molecule moves along the CNT channel smoothly as shown in (b) snapshot at 6 ps. The water molecule leaves the CNT channel at 10 ps as shown in (c).

tained due to coupling between rotational and translational motions.[15] The structure and flow of water inside a long CNT were examined using molecular dynamics.[16] It was found that, unlike continuum mechanics predictions, the flow enhancement in subcontinnum systems may not increase monotonically with decreasing flow area. A study was conducted on simulations of a water jet from a (6,6) CNT that confines water in a form of single-file molecular chain.[17] The results showed that the water forms nanoscale clusters at the outlet and they are released intermittently. A recent experimental report was on the gas and water flow measurements through microfabricated membranes in which aligned CNTs serve as pores.[18] The gas and water permeabilities of these nanotube-based membranes were observed to be several orders of magnitude higher than those of commercial polycarbonate membranes. The effects of CNT diameter on mass density, molecular distribution, and molecular orientation of water molecules inside and outside the CNTs were identified for both confined and unconfined fluids *via* molecular dynamics.[19] Recent research showed the single-file water can be transported through a (6,6) CNT driving by a bias electrostatic potential on the ends of the CNT.[20] In this work, we report a study on an energy pump by pre-twisting a small portion of a long CNT for efficient water transportation. Since it has been unveiled that the van der Waals energy between the CNT wall and the encapsulated water molecules initiates a possible motion or transportation of the molecules, the release of the pre-twisted pump will drive the water molecules and is expected to fulfill a smooth transportation of the molecules. The effect of the pump length on the efficiency of the transportation is particularly investigated, and a practical transportation of a large number of water molecules is fulfilled with the pump concept. The torsion applied to the pre-twisted portion could be realized by a practical pendulum system,[12] and hence, the realization of the energy pump is possible and practical through the design of the pendulum system.

RESULTS AND DISCUSSION

Transportation Process of One Water Molecule. The concept of an energy pump for the transportation of a water molecule by use of a CNT is described with the aid of a snapshot at 0 ps in Figure 1a. The pump is made of a portion of the CNT with several layers of carbon atoms on its two ends, shown as E1 and E2, restrained by preventing their freedoms in motion. In experiments, the restraints on E1 and E2 can be realized in experiments by the techniques of fixing a CNT as an AFM tip and/or forming an intramolecular junction as a restraint point described in refs 21 and 22. A pre-twisted angle is applied to E1 first to make the pump in a torsion buckling state, as seen in the figure. The local buckling state on the pump portion of the CNT is realized through a geometry optimization process described in the Methods. Once the prebuckling of the pump is achieved, the restraint on E2 is removed to allow the propagation of the local torsion buckling along the direction from the pump to the channel portion of the CNT, as shown in the snapshot at 6 ps in Figure 1b. It is expected that a resultant driving force by the vdW energy interacted between the CNT wall and the molecule through the propagation of the local buckling from the pump will be strong enough to initiate a possible molecular transportation.

In order to systematically investigate the feasibility and efficiency of the energy pump concept for the transportation of water molecules, seven scenarios of water transportation as shown in Table 1 are investigated. Scenario 1 is used to explore the fundamental process of the water transportation. Scenarios 2−4 focus on the effect of pump length, while scenarios 5−7 aim to elucidate the effect of environmental temperature and the fluctuations in the CNT channel. In scenarios 1−6, the environmental temperature is assumed to be 1 K to minimize the effect of thermal vibration of

TABLE 1. Simulation Details in the Research

scenarios	pump length (nm)	environmental temperature (K)	restraint on CNT channel	number of water molecule	pre-twist angle (degrees)
1	6.2	1	restrained	1	135
2	1.9	1	restrained	1	90
3	2.3	1	restrained	1	90
4	2.7	1	restrained	1	90
5	6.2	1	restrained	20	135
6	6.2	1	unrestrained	20	135
7	6.2	300	unrestrained	20	135

water molecules and carbon atoms on the transportation process.

The first scenario is on the transportation of one water molecule in a zigzag (8,0) CNT with an energy pump of the length of 4.3 nm for investigating the feasibility of the pump. The lengths of E1, E2, and the CNT channel are 1.0, 6.2, and 13.2 nm, respectively. The simulation is conducted at a temperature of 1 K. The torsion angle on E1 of the pump is 135°. A water molecule is installed at the right end of E2. In order to focus on the effectiveness of the energy pump concept, the motions of the CNT channel portion are restrained first in the simulations of the water molecule by screening out the effect of the fluctuations in the channel portion in the transportation process.

The transport process of the water molecule can be described with four stages. The first stage occurs during 0−0.8 ps starting from the unlocking of the restraint on E2. In this stage, we can see the initiation of the propagation of the local buckling on the pump or the start of the release of the potential energy stored in the pump. During this period, there are almost no momentum and resultant force on the water molecule, shown in Figure 2a,b, because the collapse of the buckling wall has not reached E2 adjacent to the water molecule. The molecule remains at its motionless state seen from the zero displacement and velocity in Figure 2c,d. The second stage starts from 0.8 ps and ends around 1.1 ps, showing a period of the interaction between the collapsed CNT wall and the water molecule and, correspondingly, the transfer of the potential energy stored in the pump to the kinetic energy of the water molecule. In the stage, the wall on the E2 portion starts to collapse around 0.8 ps due to the propagation of the buckling wall of the pump portion, and the water molecule starts moving accordingly from its static equilibrium state through the induced van der Waals potential. It is observed, from the variation of the van der Waals potential shown in Figure 2e, that there is a sharp drop, that is, from −0.55 to −2.08 eV, in the vdW energy during the period of 0.8−0.9 ps. In the second stage, an impact force in the CNT length direction with a magnitude of 0.29 nN at 0.98 ps is induced, and the momentum and velocity of the water molecule are increased from 0 to 0.09 MeV/c and 0 to 1600 m/s, respectively. The molecule is thus found to be accelerated dramatically during the short period. The third stage then follows from 1.1 to 9.5 ps, showing a steady and linear motion of the water molecule in the CNT channel, as seen in Figure 2c. The traveling distance of the molecule is about 13.2 nm in this stage. It is observed that the momentum of the water molecule remains almost constant, leading to a visually zero resultant force accompanying a constant velocity and linear displacements. The fluctuating resultant force with a mean value of zero can be attributed to the crystal structure of the CNT wall, that is, the periodic rings along the axial direction of the tube. Interestingly, the energy dissipation is found to be almost zero during the travel of the water molecule in the fixed CNT channel, showing a low friction between the water molecule and the CNT wall. The last stage describes the departure of the water molecule out of the CNT during 9.5−10 ps. In the final stage, the end of the CNT functions as a barrier[20] to the water molecule seen from small disturbances in the momentum, resultant force, and velocity of the molecules in Figure 2. Probably the doping on the carbon atoms on the end of the CNT could be necessary in reducing this barrier.

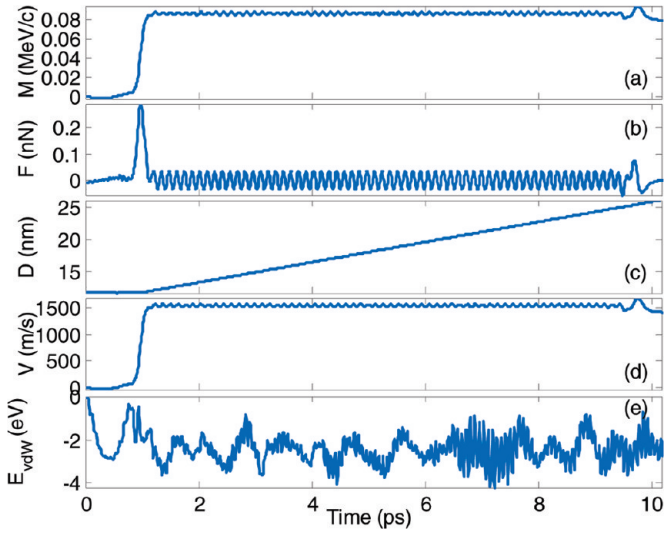

Figure 2. Transportation of one water molecule in scenario 1: (a) momentum, (b) resultant force, (c) displacement, (d) velocity of the water molecule, and (e) vdW energy of the whole system including the CNT and the water molecule.

Effect of the Pump Length on Transportation of One Water Molecule. The efficiency of the transportation is investigated with respect to the pump length in scenarios

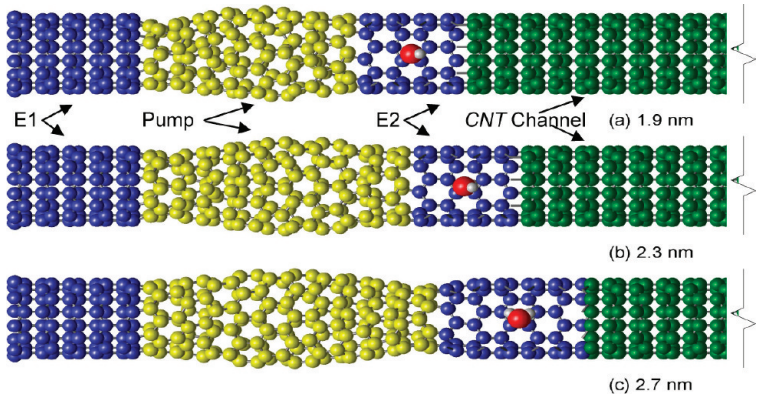

Figure 3. Effect of the pump length on the transportation of one water molecule in the zigzag (8,0) CNT channel. The lengths of E1 (blue) and E2 (blue) are 1.0 and 0.8 nm, respectively. The pump (yellow) lengths are (a) 1.9 nm, (b) 2.3 nm, and (c) 2.7 nm.

2−4. In continuum mechanics, it is known that the strain energy in a twisted bar subjected to a constant angle is inversely proportional to the length of the bar. It is therefore postulated that the length of the pump would have an impact on the transportation efficiency. In scenarios 2, 3, and 4, the pump lengths are 1.9, 2.3, and 2.7 nm, respectively, as shown in Figure 3a−c. The total length of the whole CNT is 24.8 nm, and the lengths of E1 and E2 are 1.0 and 0.8 nm. The water molecule is again located adjacent to E2.

It is observed in the simulations in Figure 4 that the water molecule immediately starts moving once the restraint on E2 is removed. The amplitude of the impact forces and durations, however, are clearly dependent on the pump sizes. For example, the durations of the impact forces, from a zero value to a peak, are around 0.14, 0.18, and 0.25 ps in the CNT with pump lengths of 1.9, 2.3, and 2.7 nm, respectively. Their corresponding peak values are 1.60, 0.88, and 0.47 nN, respectively. It is apparent that a shorter pump induces a larger force with a shorter period during the initiation of the water transportation. Such an observation is attributed to the physical interpretation that higher strain energy is stored in a shorter pump, resulting in a larger impact force (driving force). Once the water molecule enters into the CNT channel, the transportation again moves very smooth, as shown from the linear displacement and constant velocity. Because of the different impact forces at the accelerated stage, the constant velocities of the water molecule are 4450, 3480, and 2800 m/s, and consequently, the water molecules leave the end of the CNT channel at 5.1, 6.4, and 7.8 ps. From Figure 4d, it is seen that vdW potential is higher for transportation with shorter pump, which again coincides with the understanding that a shorter pump with the same pretwisted angle stores higher energy for the transportation. In our simulations, it is also observed that a water molecule cannot be transported successfully in a CNT longer than 5.0 nm with the same pretwisted angle, 90°, on E1.

Transportation of 20 Water Molecules. The feasibility of the transportation of one water molecule *via* the pump concept is demonstrated. We now investigate the transportation of 20 water molecules to further explore the practical potential of the CNT pump concept. Particularly, we focus on the effect of the environmental temperature and the fluctuations in the CNT channel portion on the transportation process. In the following scenarios 5, 6, and 7, the geometry of the pump, CNT channel, E1, and E2 and the pretwisted angle are the same as those in the first scenario. In scenarios 6 and 7, the restraint on the CNT channel portion is released. By releasing the restraint on the CNT channel, the local buckling on the pump will propagate along the CNT channel portion and will hence lead to fluctuations in the channel. Twenty water molecules are installed adjacent to E2. Snapshots at 28 ps of the molecular dynamics process for these three scenarios are shown in Figure 5a−c, while the displacement, velocity, resultant force of the water molecules, and the vdW energy be-

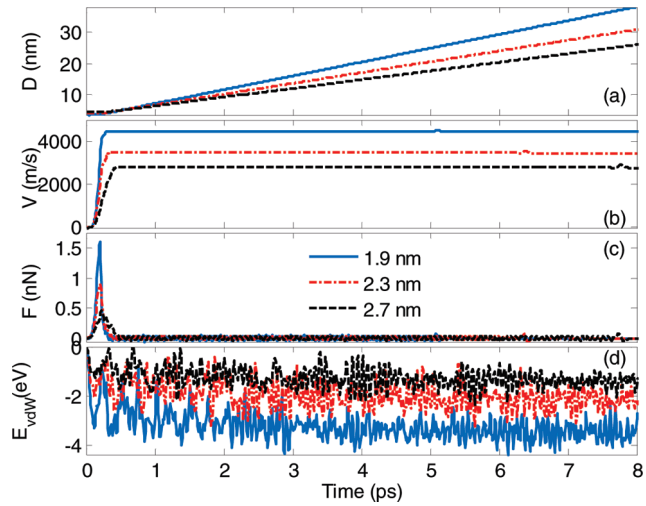

Figure 4. Transportation of one water molecule with the pump of three lengths, 1.9, 2.3, and 2.7 nm: (a) displacement, (b) velocity, (c) resultant force of the water molecule, and (d) vdW energy between the CNT and the water molecule.

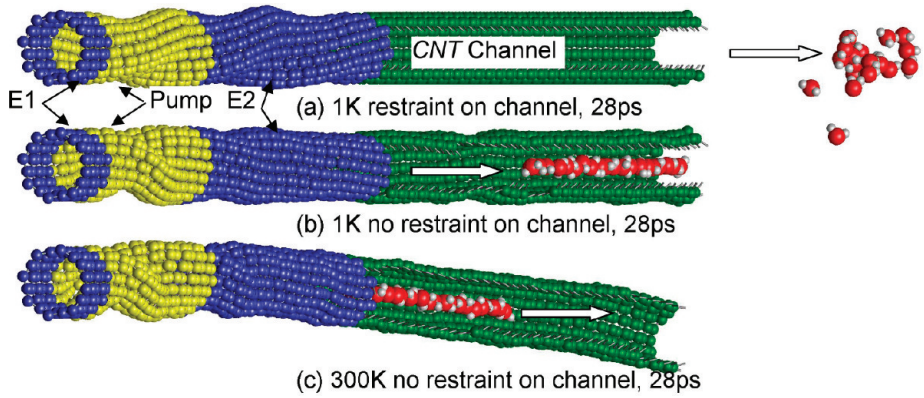

Figure 5. Snapshots on the transportation of 20 water molecules. The total length of the CNT is 24.8 nm, and the lengths of E1 (blue) and E2 (blue) are 1.0 and 6.2 nm, respectively. Twenty water molecules are installed at E2. A pretwisted angle of 135° is applied to the pump (yellow) on E1. (a) Snapshot of the fifth scenario: transportation of 20 water molecules subject to 1 K with restraint on the CNT channel; the whole process can be seen in the video attached as Supporting Information. (b) Snapshot of the sixth scenario: transportation of 20 water molecules subject to 1 K with no restraint on the CNT channel; the whole process can be seen in the video attached as Supporting Information. (c) Snapshot of the seventh scenario: transportation of 20 water molecules subject to 300 K with no restraint on the CNT channel.

tween the CNT and the molecules are provided in Figure 6a−d.

First, we will compare the results of scenarios 1 and 5 to investigate the transportation of multiple water molecules with the energy pump concept. In scenario 5, on the transportation process of the 20 water molecules, the duration of the accelerated stage is relatively longer in the processes than that in the first scenario on the transportation of one water molecule. For example, the duration is about 11.5 ps in scenario 5 before the water molecules start their smooth motion with constant velocities, whereas the duration is only about 0.3 ps in scenario 1. Two possible reasons may account for this longer accelerated period. First, 20 water molecules have higher inertia to be accelerated. Second, during the longer accelerated stage, the 20 water molecules experience more complex external resultant forces. Interestingly, in addition to the positive driving force due to the propagation of the local buckling, it is observed that the molecules experience negative driving forces, as seen in Figure 6c. Due to the negative driving force, the velocities increase non-monotonously, as seen in Figure 6b, and therefore, the transportation of the water molecules is retarded although the transportation is successful.

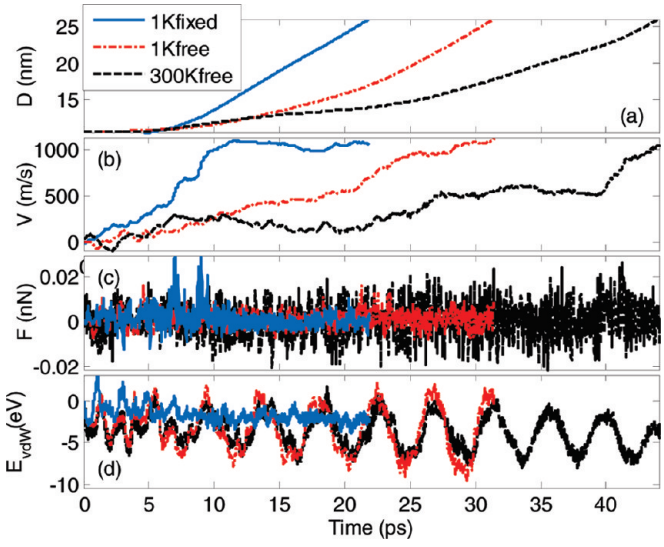

Figure 6. Effect of fluctuations of CNT channel and environmental temperature in scenarios 5, 6, and 7 on transportation of 20 water molecules: (a) displacement, (b) velocity, (c) resultant force of water molecules, and (d) vdW energy between the CNT and the water molecules.

Now, we investigate the effect of the fluctuations in the CNT channel due to the local buckling propagation from the pump on the efficiency of the transportation. The CNT channel portion is mostly unrestrained in practice. In scenarios 5 and 6, the dynamics process is at 1 K and the CNT channel is with and without restraint separately. Since the channel is without restraint in scenario 6, the fluctuations are introduced in the transportation in the scenario. It is noted that the 20 water molecules experience a faster and smoother transportation in scenario 5 than in scenario 6. Such an observation indicates that the fluctuations in CNT channel have negative effect on the water transportation. In scenario 5, the 20 water molecules are accelerated within 11.5 ps and their velocity is increased to be around 1000 m/s, followed by a smooth transportation in the restrained CNT channel. The 20 water molecules are pumped out of the CNT channel at 21.9 ps, and the snapshot at 28 ps is shown in Figure 5a. In scenario 6, however, the water molecules are accelerated in a much slower way with more fluctuation motions during the transportation. The 20 water molecules are pumped out of the CNT channel at 31.5 ps. It is understandable that in scenario 5 the potential energy is confined in the pump and E2 portion and hence results in a stronger resultant force between the CNT wall and the water molecules. However, the potential energy is distributed in the whole CNT, including the pump, E2, and the CNT channel in scenario 6, leading to a smaller resultant force on water molecules at the initial pumping

process, as shown in Figure 6c. In addition, the magnitude of the vdW energy is generally larger in scenario 5 at the initial pumping stage than in scenario 6, indicating that more potential energy dissipates during the transportation when the restraint on the CNT channel is released. Besides, due the fluctuations in the CNT channel, the water molecules experience larger transverse and torsion motions that will definitely induce more friction between the CNT and water molecules and accordingly retard the transportation further. The effect of the transverse motions will also be discussed next when the environmental temperature effect is investigated.

Finally, we investigate the thermal effect on the transportation from the comparison between scenarios 6 and 7. The higher environmental temperature, 300 K, in scenario 7 causes stronger water molecule motion, which results in increased collisions between water molecules and the CNT channel in both transverse and longitudinal directions and, therefore, leads to a more severe fluctuating unbalanced force in the transverse direction of the tube, as shown in Figure 6c. On the contrary, at a lower temperature (*i.e.*, 1 K in scenario 6), only a less fluctuating force would be induced. Therefore, the velocities of the water molecules in scenario 7 are accelerated even slower than in scenario 6, resulting in a longer transportation process (*i.e.*, 43.8 ps). It is observed that, after 10.5 ps, the velocities of the water molecules in scenario 7 are lower than those in scenario 6, indicating an obviously slower increase in the velocities of the molecules at the higher temperature, or more friction initiated between the CNT wall and the molecules. In our simulations, the transportation of the 20 molecules becomes impossible when the system is subjected to a temperature of 1500 K. Further endeavors on an efficient transportation at higher environmental temperature are underway in our research group.

CONCLUSION

In summary, we have performed molecular dynamics simulations on the transportation of water molecules with the introduction of an energy pump concept. It is demonstrated that a water molecule can be successfully accelerated in a CNT channel with the pump concept. Moreover, the water molecule is found to move smoothly in the CNT channel before leaving the end of the CNT that is found as a barrier to the water molecule. A faster and more efficient transportation of the water molecules is identified with an application of a shorter pump as more energy is found to be stored in the shorter pump than its longer counterpart. In the transportation of 20 water molecules, it is observed that the accelerated duration is higher than that in the transportation of single water molecule due to higher inertia of multimolecules. In addition, higher environmental temperature and fluctuations in the CNT channel due to buckling propagation will all lead to lower water velocities and hence retard the transportation process.

METHODS

The atomic interaction is modeled by the COMPASS force field (condensed-phased optimized molecular potential for atomistic simulation studies),[23,24] which is the first *ab initio* force field that was parametrized and validated using condensed-phase properties. This force field has been proven to be applicable in describing the mechanical properties of carbon nanotubes.[25,26] In the COMPASS force field, the total potential energy, E, is expressed as follows:[23]

$$E = \begin{aligned} &\sum E^{(b)} + \sum E^{(\theta)} + \sum E^{(\phi)} + \sum E^{(\chi)} + \\ &\sum E^{(bb')} + \sum E^{(b\theta)} + \sum E^{(b\phi)} + \\ &\sum E^{(b'\phi)} + \sum E^{(\theta\theta')} + \sum E^{(\theta\phi)} + \\ &\sum E^{(\theta\theta'\phi)} + \sum E^{(\mathrm{vdW})} + \sum E^{(\mathrm{elec})} \end{aligned} \quad (1)$$

where b and b' are the lengths of two adjacent bonds, θ and θ' are the adjacent two-bond angles, ϕ is the dihedral torsion angle, and χ is the out of plane angle. The total potential energy may be divided into two categories, namely, (i) contributions from each of the internal valence coordinates (*i.e.*, $\sum E^{(b)}$, $\sum E^{(\theta)}$, $\sum E^{(\phi)}$, and $\sum E^{(\chi)}$); and (ii) cross-coupling terms between internal coordinates (*i.e.*, $\sum E^{(bb')}$, $\sum E^{(b\theta)}$, $\sum E^{(b\phi)}$, $\sum E^{(b'\phi)}$, $\sum E^{(\theta\theta')}$, $\sum E^{(\theta\phi)}$, and $\sum E^{(\theta\theta'\phi)}$); and (iii) nonbonded interactions (*i.e.*, the van der Waals energy, $\sum E^{(\mathrm{vdw})}$, and the Coulomb electrostatic energy, $\sum E^{(\mathrm{elec})}$). It should be noted that the vdW energy is represented by a sum of repulsive and attractive Lennard-Jones terms.[27]

Molecular dynamics simulations involve an initial geometry optimization process (using the conjugate-gradient method) for the pump portion while restraining the motions of E1 and E2 portions. Once the minimization process is completed, the CNT with the twisted pump and water molecule(s) are subjected to an NVT ensemble (*i.e.*, constant volume and constant temperature dynamics) simulation process for 100 ps at a prescribed temperature during which the entire system reaches a thermodynamic equilibrium. A NVE (*i.e.*, constant volume/constant energy dynamics) simulation process of another 100 ps will be followed by releasing the E2 to initiate the motion of water molecule(s). The Verlet velocity algorithm[28] is adopted in the NVE simulation to integrate the motion of equations for the whole system. All discussions in the present research are only focused on this NVE process, and the incremental step in the dynamics simulations is chosen to be 1.0 fs.

The amount of momentum that water molecules possess can be calculated by taking the product of two physical quantities: the mass and the velocity of the water molecules. The velocity of 1/20 water molecules is calculated as the velocity on the center of mass. According to Newton's second law, the rate of change of the momentum of the water molecule is proportional to the resultant force on the water molecule. Therefore, through a calculation of the derivative of the momentum with respect to the time, the resultant force applied to water molecules can be obtained.

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Supporting Information Available: Transportation process of 20 water molecule in scenarios 5 and 6 are provided in two videos. This material is available free of charge *via* the Internet at http://pubs.acs.org.

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