


## Mechanical activation of DNA transport across single-walled carbon nanotubes

Junjie Gao(高俊杰), Yichao Wu(吴逸超), Siqi Yu(俞斯棋), Xiaoyan Zhou(周晓艳), and Hangjun Lu(陆杭军)
**Citation:**Chin. Phys. B, 2025, 34 (**10**): 108701. DOI: 10.1088/1674-1056/adce9b
http://cpb.iphy.ac.cn; http://iopscience.iop.org/cpb

**What follows is a list of articles you may be interested in**

---

## Reconfiguration of B-DNA structure induced by ethanol

Yue Huang(黄悦), Yipeng Chen(陈以鹏), Jing Li(李静), Rongri Tan(谈荣日), and Huanhuan Qiu(邱环环)
Chin. Phys. B, 2025, 34 (**8**): 088707. DOI: 10.1088/1674-1056/adbed9

## Single-molecule investigation of the impacts of fluorescent DNA-binding proteins on DNA mechanical properties

Yaxi Cheng(成雅茜), Shang Gao(高上), Xianqi Ye(叶贤其), Chuang Tan(谭创), and Jie Ma(马杰)
Chin. Phys. B, 2025, 34 (**8**): 088702. DOI: 10.1088/1674-1056/addcbd

## Effect of mono-/divalent metal ions on the conductivity characteristics of DNA solutions transferring through a microfluidic channel

Jie Zhu(朱洁), Jing Xue(薛菁), Wei Zhao(赵伟), Chen Zhang(张琛), Xiaoqiang Feng(冯晓强), and Kaige Wang(王凯歌)
Chin. Phys. B, 2023, 32 (**11**): 118704. DOI: 10.1088/1674-1056/acfaf6

## Heterogeneous hydration patterns of G-quadruplex DNA

Cong-Min Ji(祭聪敏), Yusong Tu(涂育松), and Yuan-Yan Wu(吴园燕)
Chin. Phys. B, 2023, 32 (**2**): 028702. DOI: 10.1088/1674-1056/ac7452

## Adsorption dynamics of double-stranded DNA on a graphene oxide surface with both large unoxidized and oxidized regions

Mengjiao Wu(吴梦娇), Huishu Ma(马慧姝), Haiping Fang(方海平), Li Yang(阳丽), and Xiaoling Lei(雷晓玲)
Chin. Phys. B, 2023, 32 (**1**): 018701. DOI: 10.1088/1674-1056/ac5c3a

---

# Mechanical activation of DNA transport across single-walled carbon nanotubes

Junjie Gao(高俊杰), Yichao Wu(吴逸超), Siqi Yu(俞斯棋), Xiaoyan Zhou(周晓艳)[†], and Hangjun Lu(陆杭军)[‡]

*Department of Physics, Zhejiang Normal University, Jinhua* 321004, *China*

(Received 19 February 2025; revised manuscript received 12 April 2025; accepted manuscript online 21 April 2025)

We employed molecular dynamics simulations to investigate the directed transport of a double-stranded oligonucleotide (dsDNA) through a single-walled carbon nanotube (SWNT) powered by external mechanical vibrations. It is thermodynamically favorable for dsDNA to adsorb inside the SWNT, and its transport through the nanotube is challenging due to the high energy barrier. However, we demonstrate that mechanical vibrations at specific frequencies can effectively drive the dsDNA through the nanotube based on a ratchet effect. The system is driven away from thermal equilibrium, and the spatial inversion symmetry is broken by mechanical vibrations. This study provides valuable insights into the mechanisms of mechanically activated DNA transport and highlights the potential of using SWNTs as nanoscale conduits for dsDNA delivery in nanobiotechnology and biomedicine.

**Keywords:** double-stranded oligonucleotide (dsDNA), single-walled carbon nanotube (SWNT), mechanical vibrations, ratchet effect

**PACS:** 87.14.gk, 87.15.ap, 87.85.Rs, 05.40.–a

**DOI:** 10.1088/1674-1056/adce9b **CSTR:** 32038.14.CPB.adce9b

## 1. Introduction

The ability to manipulate biomolecules transport through nanopores is crucial for both fundamental biological processes and broad applications in various scientific and technological fields.[1–11] One of the most intriguing applications is the directed transport of nucleic acid molecules, such as DNA and RNA, through nanopores like carbon nanotubes (CNTs) and graphene nanopores, which holds significant promise for nanobiotechnology and biomedicine.[12–14] DNA-based nanomaterials can be engineered to transport drugs, genes, and other therapeutic agents to specific cellular sites.[15] Additionally, nanopores have been utilized for DNA sequencing, serving as a powerful tool that offers rapid readout, single-molecule sensitivity, and long read lengths.[4,16]

Recent advancements in nanotechnology have led to the exploration of various nanoscale conduits for DNA transport, with solid-state nanopores emerging as promising candidates. Carbon nanotubes, featuring unique structures and exceptional properties, have been widely used as models to study complex biological phenomena, such as the gating effects of water channels,[17,18] and ion channel selectivity.[19,20] When organized into hexagonally packed two-dimensional arrays, carbon nanotubes provide simple and potentially more robust platforms for investigating the fundamental mechanisms of membrane translocation.[3,13] Yeh and Hummer investigated the translocation of single-stranded RNA molecules through carbon nanotube membranes and discovered that the unique conformational flexibility and hydrophobicity of RNA result in sequence-dependent translocation.[13] Gao *et al.* further studied the translocation dynamics of single-stranded DNA (ssDNA) molecules through a polarized nanotube membrane under an applied electric field.[3] Geng *et al.* investigated the spontaneous incorporation of short CNTs into lipid bilayers and live cell membranes to form channels, termed CNT porins, which exhibit robust transport properties for ions, water, and DNA. The CNT porins display stochastic gating behavior and ion selectivity, making them a promising platform for biomimetic applications, including synthetic cells, drug delivery, and biosensing.[21] Liu *et al.* discovered that the electrophoretic transport of small ssDNA oligomers through carbon nanotubes is characterized by significant transient increases in ion current. This finding potentially paves the way for more precise control of DNA translocation across membranes.[22] By applying constant or alternating biasing voltages, Luan *et al.* found that the dsDNA molecule can be unzipped at the junction of the Y-shaped carbon nanotube.[23]

Over the past decades, progress has been made in the transport of materials within carbon nanotubes, primarily achieved through the application of chemical gradients,[24] thermal gradients,[25–27] external electric fields,[28–34] and vibrating charges.[35,36] In addition, various mechanical methods have been suggested to facilitate the pumping of water through CNTs capitalizing on the excellent mechanical properties of these nanotubes.[37–40] Recently, we have demonstrated that the "nanobubble" trapped in the nanotube can be

[†]Corresponding author. E-mail: zxylu@zjnu.cn

[‡]Corresponding author. E-mail: zjlhjun@zjnu.cn

© 2025 Chinese Physical Society and IOP Publishing Ltd. All rights, including for text and data mining, AI training, and similar technologies, are reserved.

removed conveniently by water flow powered by mechanical resonance.[41]

Despite these advances, the mechanical transport of more complex biomolecules, such as dsDNA, remains challenging due to the high energy barriers involved. While it is thermodynamically favorable for dsDNA to adsorb inside SWNTs, its transport through the nanotube is impeded by these barriers. Given these challenges, the question arises: Is it possible to achieve the transport of more complex biomolecules using a nanopump driven by mechanical perturbations?

In this study, we investigate the dynamics of dsDNA oligonucleotide transport through a vibrating SWNT using all-atom molecular dynamics (MD) simulations. Our simulations revealed that mechanical vibrations at specific frequencies can effectively drive dsDNA through the nanotube based on a ratchet effect. This mechanism involves breaking the spatial inversion symmetry and driving the system away from thermal equilibrium, thereby facilitating the transport of dsDNA despite the high energy barriers involved. We examined the conformational changes of the DNA oligonucleotide and the interactions between the DNA and the walls of the SWNT. Both water molecules and the dsDNA confined within the SWNT gain significant kinetic energy from the mechanical resonance, which facilitates their transport.

## 2. Computational details

The simulation framework is illustrated in Fig. 1. An uncapped (20,20) armchair SWNT with a length of 10 nm and a diameter of 2.7 nm is embedded along the $z$-axis between two carbon planes, which form an artificial membrane separating bulk water into two sides. The membrane and the atoms at the bottom part of the SWNT (shown in black) are all fixed at their original positions during the simulation. A dsDNA fragment with ten base pairs and the sequence CCGCTAGCGG is initially encapsulated in the center of the SWNT, surrounded by water molecules. The length of dsDNA fragment is approximately 4 nm. As in our previous studies,[42] a carbon atom near the left end of the SWNT (referred to as the "driving atom" and shown in red in Fig. 1) is set to undergo periodic simple harmonic motion along the $y$-axis. The motion of the driving atom follows the equation $y = y_0 - A\sin(2\pi ft)$, where $y_0$ is the equilibrium position, the amplitude $A$ is 0.18 nm, and $f$ is the vibration frequency.

All simulations were performed using the GROMACS 2016.5 software package in the NVT ensemble with the initial box size dimensions of $L_x = 5.2$ nm, $L_y = 5.2$ nm, $L_z = 17$ nm. Periodic boundary conditions are applied along all three axis directions. The temperature is maintained at 300 K using the velocity-rescale thermostat algorithm. The equations of motion are integrated using the leapfrog algorithm with a time step of 1.0 fs. A total of 7695 water molecules were added to the system. The SPC model was selected to simulate water molecules. Since the DNA molecule carries a certain amount of negative charge ($-18e$), 18 $Na^+$ ions were added to the aqueous region to neutralize the system.

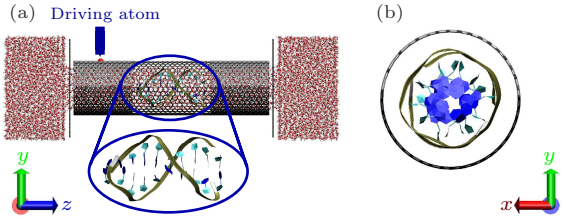



**Fig. 1.** Schematic diagram of the simulation system. (a) Snapshot of the simulation system. Two reservoirs are connected by an uncapped (20, 20) SWNT combined with two carbon planes. The red and white spheres represent the oxygen and hydrogen atoms in water molecules, respectively. The vibrating atom of the SWNT oscillates periodically along the $y$-axis. Lower panel: enlarged side view of the dsDNA confined within the SWNT. (b) Top view of the simulation system along the $z$-axis. The carbon planes and water molecules are omitted for clarity, showing only the dsDNA and the SWNT.

The AMBER99sb force field was used to describe the atomic interactions in dsDNA and the interactions between the atoms in dsDNA and water molecules or ions. The SPC model was employed for water molecules. The carbon nanotube is regarded as a large molecule. The total potential energy function of CNT can be expressed in the following form:

$$\begin{aligned} V_{\text{total}} = & \sum_{\text{VDW}} 4\varepsilon_{\text{CC}} \left[ \left( \frac{\sigma_{\text{CC}}}{r} \right)^{12} - \left( \frac{\sigma_{\text{CC}}}{r} \right)^{6} \right] \\ & + \sum_{\text{bonds}} \frac{1}{2} k_{\text{b}} (r - r_0)^2 + \sum_{\text{angles}} \frac{1}{2} k_\theta (\theta - \theta_0)^2 \\ & + \sum_{\text{dihedrals}} \frac{1}{2} k_\xi (r - r_\xi)^2, \end{aligned}$$

where $\varepsilon_{\text{CC}} = 0.3612$ kJ/mol, $\sigma_{\text{CC}} = 0.34$-nm bond length of $r_0 = 0.142$ nm, bond angle of $\theta_0 = 120^\circ$, the spring constant of $k_{\text{b}} = 393960$ kJ·mol$^{-1}$·nm$^{-2}$, and $k_\theta = 527$ kJ·mol$^{-1}$·deg$^{-2}$, $k_\xi = 52.718$ kJ·mol$^{-1}$·deg$^{-2}$. Long range electrostatic interactions with a cutoff for real space of 1.4 nm were computed by using a particle-mesh Ewald method. The cutoff distance for the short-range van der Waals forces is also set at 1.4 nm.

The simulation begins with an energy minimization process. During the initial equilibration process, all carbon atoms in the SWNT and the CNPs were fixed, and a harmonic potential was applied to restrain the dsDNA, preventing the system from collapsing due to initial unreasonable forces. The system was equilibrated for 20 ns. During this period, the dsDNA strand undergoes a thermalization process and settles into its equilibrium position. Following the equilibration process, we tracked the movement of each atom during the last 30 ns and collected data for further analysis.

We also performed computer simulations of a system without water molecules. Based on the original system, all water molecules are removed and a harmonic potential is applied to the dsDNA molecule for 20 ns of equilibration. During this process, $Na^+$ ions could spontaneously move and eventually

adsorb onto the dsDNA surface. Subsequently, we introduced mechanical vibrations with frequencies set at 1200 GHz and 1000 GHz and conducted a 30-ns computer simulation after removing the constraints on the DNA.

## 3. Result and discussion

Previous studies have shown that DNA can be adsorbed inside carbon nanotubes with appropriate diameters due to van der Waals interactions.[12,43] In our previous work, we demonstrated that water within a carbon nanotube can be efficiently driven by external mechanical vibrations.[42,44] Thus, interesting questions arise. Can mechanical vibrations drive the transport of DNA? Will DNA molecules become blocked inside the carbon nanotube?

To address these questions, we analyzed the trajectories of the center of mass (CoM) of the dsDNA inside the carbon nanotube under external vibrations at different frequencies, with the results shown in Fig. 2. Without external vibration ($f = 0$ GHz), the dsDNA remains relatively stable near its initial position ($z = 8.5$ nm) (see Fig. 2(a)). When external mechanical vibrations are introduced, the dsDNA inside the SWNT is disturbed. The CoM of the dsDNA deviates from the central position but does not escape the SWNT due to the barrier at the outlet. The nanotube's outlet is located at $z = 13.5$ nm, marked by the dashed line in Fig. 2(a). When the vibration frequency is increased to 1000 GHz, the dsDNA escapes from the carbon nanotube. At 1200 GHz, the dsDNA is ejected from the carbon nanotube in the shortest amount of time (about 5 ns). However, when the frequency increases further, the dsDNA is blocked at the outlet and cannot escape. This phenomenon indicates that higher vibration frequencies do not necessarily enhance transport efficiency; in fact, excessively high frequencies can hinder directed transport. This finding aligns with previous studies on nanopumps transporting water, where transport efficiency also exhibits a peak response to frequency.

We further analyzed the probability distribution of dsDNA translocation time at frequency 1200 GHz. We varied the initial conditions and performed 10 simulations of 15 ns, then statistically analyzed the translocation time to obtain the probability distribution. We found that the time for dsDNA to pass through the carbon nanotube exhibits some fluctuations, but there are no deviations of several orders of magnitude. The value with the highest probability distribution is around 5 ns.

Figure 2(b) shows snapshots of the system after 30 ns of simulations. It is observed that at vibration frequencies of 1000 GHz and 1200 GHz, dsDNA can be transported out of the nanotube into the external reservoir. At 1500 GHz and 2000 GHz, dsDNA can be transported to the vicinity of the nanotube's opening. Our simulation results show that at specific frequencies, dsDNA can be efficiently driven through the carbon nanotube by external mechanical vibrations. However, dsDNA cannot be driven out the carbon nanotube without water (shown in Fig. 2(c)). Our simulation results indicate that water plays a key role and relying solely on mechanical waves is insufficient to transport dsDNA through the CNT effectively.

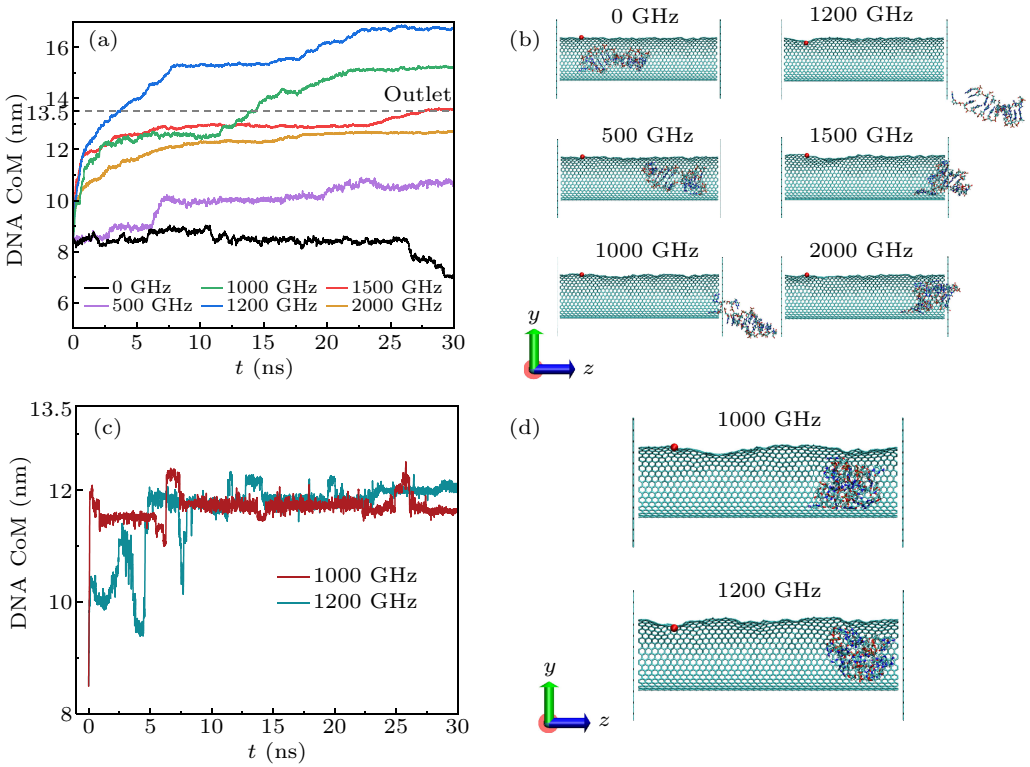



**Fig. 2.** (a) The trajectories of the center of mass (CoM) of the DNA molecule. (b) Final snapshot of the simulated system (water molecules and ions are omitted for clarity). (c) The trajectories of the center of mass (CoM) of the DNA molecule in vacuum. (d) Final snapshot of the simulated system in vacuum.

The van der Waals interactions between dsDNA and SWNT play a key role in the transportation of dsDNA, which facilitates the spontaneous entry of DNA into the CNT but acts as a hindrance to its exit. In a study by Wei Min *et al.* on nitrogen gas nanobubbles in CNTs, it was found that expelling nitrogen gas nanobubbles from the nanotube also requires overcoming an energy barrier.[41]

Here, we calculated the van der Waals interaction energy between dsDNA and the SWNT for each group, as shown in Fig. 3. The Lennard–Jones (L–J) potential is used to describe the van der Waals interactions. The DNA–CNT interaction energy is calculated using the formula

$$V_{\mathrm{L-J}} = \sum_{ij} 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right],$$

where $\varepsilon$ and $\sigma$ are the depth and width of the potential well, respectively, and $r_{ij}$ is the distance between the $i$-th atoms in the DNA and the $j$-th carbon atoms in the CNT. In this study, the cutoff radius for the L–J interaction is set to 1.4 nm.

In the control group where the frequency is 0 GHz, DNA molecules tend to stay in the middle of the SWNT. To calculate the interaction energy profile along the nanotube, the DNA is pulled from $z = 8.5$ nm to $z = 15.5$ nm. The red dashed line represents the result of polynomial fitting. From Fig. 3, we can see that the lowest interaction energy locates in the middle of the SWNT. The van der Waals interaction energy increases with the distance from the center of the carbon nanotube and ultimately tends towards zero, forming a U-shaped potential energy curve that is low at the center inside the carbon nanotube and high at both ends.

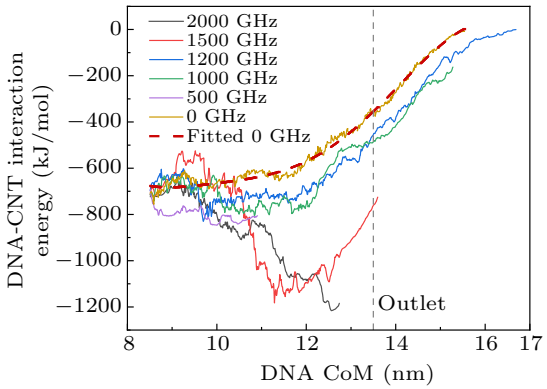



**Fig. 3.** The interaction energies between DNA and CNT vary with the $z$ position of the CoM of DNA for different vibration frequencies.

When external mechanical vibrations are introduced, the shape of the interaction energy curve changes. When $f =$ 500 GHz, the interaction energy is lower in the region close to the right end of the carbon nanotube (CoM of dsDNA in the range of 8.8 nm to 11 nm) compared to the control group. By the end of the simulation, the dsDNA is trapped in this region (see Fig. 2(b)). Interestingly, when $f = 1500$ GHz, the interaction energy curve undergoes a significant change, particularly at the ends of the carbon nanotube. A new potential well forms in this region, with the lowest interaction energy located at approximately $z = 11.5$ nm. Notably, the dsDNA length is 4 nm in our simulations, and the end of the CNT is at $z = 13.5$ nm, meaning the right end of the dsDNA aligns with the right end of the CNT. Furthermore, when $f = 2000$ GHz, the lowest interaction energy is at $z = 12.5$ nm. We observed significant changes in the morphological structure of the DNA (as shown in Fig. 2(b)). The snapshots reveal that the DNA has visibly shortened in length and has accumulated near the tube opening, with a small part protruding beyond the end of the CNT. In this case, the driving force is insufficient for water to push the dsDNA out of the CNT. For frequencies of 1200 GHz and 1000 GHz, dsDNA can be transported through the SWNT driven by external mechanical vibrations. The shape of the interaction energy between the dsDNA and the SWNT is similar to that of the control group, but it is lower overall.

Our simulations reveal that the geometrical structure of the SWNT is modified by external mechanical vibrations, which in turn excite complex mechanical waves. As a result, the distance between the dsDNA and the SWNT wall fluctuates, leading to changes in the profile of their interaction energy. To further investigate this phenomenon, we calculated the number of atoms in dsDNA, excluding hydron atoms, within a specific region near the SWNT wall, where the distance ranges from 0.34 nm to 0.5 nm. These atoms are called contacting atoms in this paper. The results of this analysis are presented in Fig. 4.

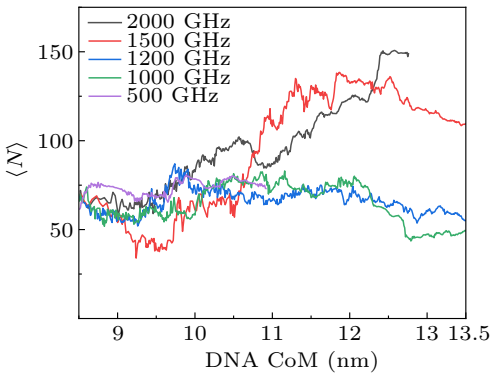



**Fig. 4.** The number of atoms in dsDNA, excluding hydrogen atoms, within a region where the distance to the SWNT wall ranges from 0.35 nm to 0.5 nm.

As shown in Fig. 4, we found that for $f = 1000$ GHz and $f = 1200$ GHz, the structure of dsDNA is relatively stable, with little change in the number of contacting atoms $\langle N \rangle$. When the CoM of the DNA approaches the nanotube opening, part of the dsDNA has already moved out of the SWNT, resulting in a decrease in the number of contacting atoms. However, for vibration frequencies of 2000 GHz and 1500 GHz, when CoM of the DNA moves to a position near 10.511 nm, the

DNA is compressed and its shape changes, leading to a significant increase in the number of atoms in contact with the CNT. This causes a further decrease in potential energy in the range of 11 nm–13 nm, forming a potential well.

Furthermore, we consider what factors lead to the directional transport of dsDNA and why dsDNA can overcome the energy barrier to reach the aqueous environment at specific vibration frequencies, while at some other frequencies, DNA can only be transported to the nanotube opening. Since dsDNA directly interacts only with water molecules and the SWNT, their dynamical behavior is closely related. The external mechanical disturbance can cause the nanotube wall to vibrate and generate waves that propagate outward. According to our previous studies,[42,45] we know that these vibrations can transfer mechanical energy to the water molecules inside the nanotube, resulting in an uneven spatial distribution of energy among the water molecules. This, in turn, can induce directional transport of water molecules, thus realizing the function of a nanoscale water pump. For such a nanoscale water pump, there exists a specific frequency at which the system can achieve mechanical resonance, maximizing the water flow rate. The water flow rate is an important measure of the transport capacity of the nanoscale water pump. Therefore, we calculated the water flow rate for all systems and plotted it in Fig. 5.

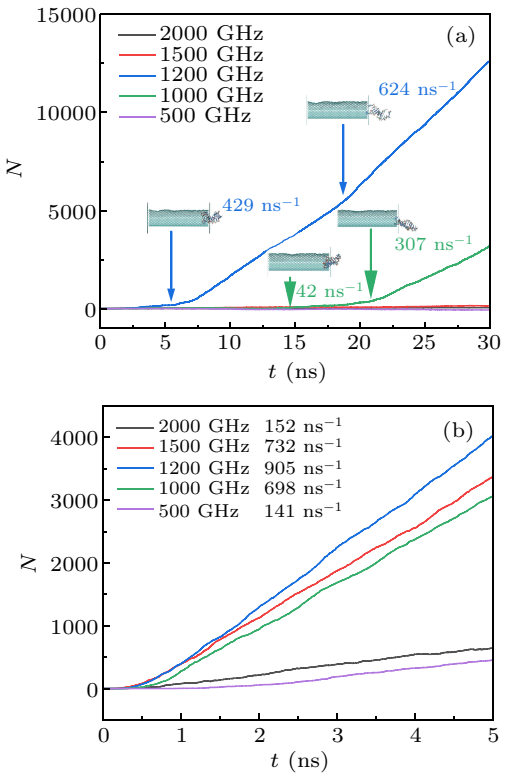



**Fig. 5.** The net number of water molecules passing through the SWNT over time for system with dsDNA (a) and system without dsDNA (b).

The difference between the number of water molecules entering from the left end and exiting from the right end, and those entering from the right end and exiting from the left end, is depicted in Fig. 5. The net flux of water through the carbon nanotube is defined here as the number of water molecules moving from the left side of the carbon nanotube to the right side per unit time, minus the number of water molecules moving from the right side of the carbon nanotube to the left side per unit time. When there are no DNA molecules blocking the carbon nanotube, due to thermal motion, water molecules can move from the left side to the right side and also from the right side to the left side of the carbon nanotube. The water flux behavior can be divided into three distinct phases for the cases of 1000 GHz and 1200 GHz. During the initial period (0 ns–7 ns for 1000 GHz and 0 ns–15 ns for 1200 GHz), the majority of the dsDNA molecule resides inside the SWNT, effectively blocking the passage of water molecules. This period is designated as phase I: the clogging phase. As the DNA molecule moves to the right end and partially exits the SWNT, an increasing number of water molecules begin to pass through the SWNT. This transition period is referred to as phase II: the partial clogging phase (occurring from 7 ns to 20 ns for 1200 GHz and from 15 ns to 22 ns for 1000 GHz). During this phase, although a portion of the DNA still remains within the SWNT, the obstruction is gradually alleviated, allowing more water molecules to flow through. Finally, phase III: the unobstructed phase, begins after 20 ns for the 1200-GHz case and after 22 ns for the 1000-GHz case. In this phase, the DNA molecule has almost entirely exited the SWNT, resulting in the highest water flux achievable for the nanoscale pump at the respective frequency, which corresponds to the steepest slope of the flux curve.

Notably, during phase III, the net number of water molecules passing through the CNT per unit time (i.e., the water flux) is higher for the 1200-GHz case than for the 1000-GHz case. This indicates that the transport capacity of the nanoscale pump is greater at 1200 GHz than at 1000 GHz. This observation is consistent with the transport efficiency of the dsDNA molecule shown in Fig. 1 for these two frequency cases. Interestingly, our simulation results indicate that the dsDNA molecule cannot be pumped out of the nanotube in the absence of water (see Fig. 1(c)).

For vibration frequencies of 500 GHz and 2000 GHz, the net flux of water molecules through the SWNT is very low even in the absence of dsDNA inside the nanotube (see Fig. 5(b)). In these two cases, the mechanical energy of the vibrating carbon atoms cannot be effectively transferred to the water molecules or the dsDNA molecule inside the nanotube. Consequently, the pumping efficiency is extremely low. The dsDNA molecule is encapsulated within the nanotube, and the water molecules are completely blocked.

To better characterize the role of water in the transport of DNA, we analyzed the average kinetic energy of water molecules within a 2-nm range on both the left and right sides of the DNA at typical frequencies of 500 GHz, 1000 GHz,

and 1200 GHz, as shown in Fig. 6. The difference in average kinetic energy between the two sides reflects the pressure difference on either side of the dsDNA. The greater the difference in average kinetic energy, the shorter the time required for dsDNA to be transported to the tube outlet, and the higher the transport efficiency. As indicated in Fig. 6, the water molecules on the left side of the dsDNA exhibit greater kinetic energy than those on the right side. This is attributed to the fact that the mechanical vibration of the CNT is more pronounced near its left end. At frequencies of 1000 GHz and 1200 GHz, the difference in the average kinetic energy of water molecules between the two sides is significant. However, at 500 GHz, the difference is relatively weak. This is because 1000 GHz and 1200 GHz are closer to the resonance frequency of the carbon nanotube (CNT), while 500 GHz is far from the resonance region. Therefore, at frequencies of 1000 GHz and 1200 GHz, the carbon nanotubebased nanopump exhibits superior transport efficiency for dsDNA, which is in good agreement with the results shown in Fig. 5(a).

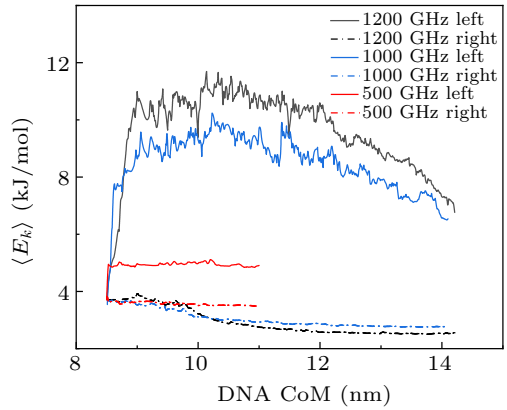



**Fig. 6.** The average kinetic energy of water molecules within a 2-nm range on both the left and right sides of the dsDNA under typical frequencies.

The impact of mechanical vibrations on the structure of DNA during its transit through the SWNT was assessed using RMSD as a measure. RMSD provides a quantitative assessment of the deviation of the DNA molecule's structure from its initial conformation, which can be indicative of structural changes or stability under the influence of mechanical vibrations. The variations in RMSD values were calculated as a function of the CoM of the dsDNA molecule, as depicted in Fig. 7. This analysis helps to understand how mechanical vibrations affect the integrity and conformation of DNA molecules during transport through nanoscale environments, which is crucial for applications in nanotechnology and molecular biology.

At 1200 GHz, the nanoscale pump exhibits the strongest transport capability for dsDNA. However, it is observed that the RMSD value of dsDNA is at its lowest compared to other cases. The RMSD value of dsDNA shows an inverse relationship with the transport capacity of the nanochannel. The relatively high RMSD values near the tube opening for the 2000-GHz and 1500-GHz cases further corroborate the previously mentioned fact that the dsDNA molecules in these two groups undergo more significant morphological changes near the tube opening.

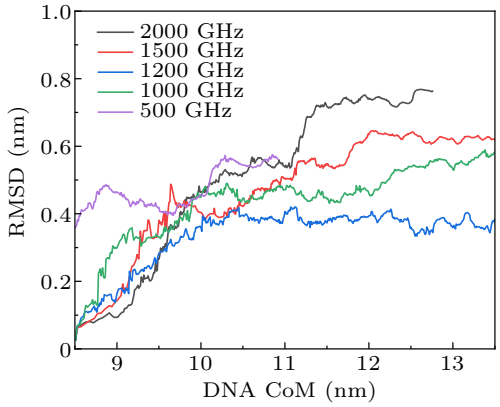



**Fig. 7.** The RMSD of DNA as a function of the position of the DNA centroid.

We also simulated the transport behavior of dsDNA by carbon nanotubes of different sizes and chiralities, and the transport behavior of ssDNA. It was found that the main transport behavior of biomolecules confined in carbon nanotubes has certain similar laws when driven by non-equilibrium mechanical vibration. For a specific carbon nanotube system, there exists a specific resonance frequency. When the carbon nanotube vibrates near the resonance frequency, it has a better transport effect on biomolecules.

Indeed, the frequencies used in our simulations (1000 GHz–2000 GHz) fall within the terahertz range, which currently exceeds the operating capabilities of conventional RF devices. However, these frequencies correspond to the natural resonance frequencies of (20,20) SWNT. The natural frequency of SWNTs is strongly dependent on their dimensions, larger SWNTs exhibit lower resonance frequencies. We performed molecular dynamics simulations on the (25,25) SWCNT system and calculated its natural frequency to be approximately 400 GHz. The resonance frequency of the original (20,20) SWNT in the system was about 1000 GHz. The resonance frequency significantly decreased when the diameter of the SWCNT changed from 2.70 nm to 3.39 nm. Therefore, by tuning the size of the SWNTs, it is possible to shift the resonance frequency toward more experimentally accessible ranges, making practical implementation more feasible.

## 4. Conclusions

In this study, we have investigated the mechanisms of mechanically activated dsDNA transport through SWNT using all-atom molecular dynamics simulations. Our results demonstrate that external mechanical vibrations at specific frequencies can effectively drive dsDNA through the nanotube, over-

coming the high energy barriers that typically impede its transport. This phenomenon is attributed to the ratchet effect induced by the mechanical vibrations, which breaks the spatial inversion symmetry and drives the system away from thermal equilibrium.

We found that the transport efficiency of dsDNA is highly dependent on the vibration frequency. At 1200 GHz, the dsDNA was transported out of the nanotube most efficiently, while away from the resonance frequency regions (e.g., 1500 GHz and 2000 GHz) led to partial blockage at the nanotube opening. This suggests that excessive vibration frequencies may disrupt the directional transport. The profile of the interaction energy between the dsDNA and the SWNT is also altered. Additionally, our simulations revealed that water molecules play a crucial role in facilitating the transport of dsDNA. In the absence of water, the dsDNA could not be effectively driven out of the nanotube, indicating that the mechanical vibrations alone are insufficient for efficient transport.

The interaction energy analysis showed that the van der Waals forces between the dsDNA and the SWNT significantly influence the transport process. The formation of potential wells near the nanotube opening at certain vibration frequencies (e.g., 1500 GHz) further highlights the complex interplay between mechanical vibrations and molecular interactions. Furthermore, the structural integrity of dsDNA during transport was assessed by calculating the RMSD of the DNA molecule. We found that higher transport efficiency at 1200 GHz was associated with lower RMSD values, suggesting minimal structural deformation of the DNA during transport.

In summary, our study provides valuable insights into the mechanisms underlying mechanically activated DNA transport through SWNTs. The findings highlight the potential of using SWNTs as nanoscale conduits for biomolecular delivery in nanobiotechnology and biomedicine.

## Acknowledgement

Project supported by the National Natural Science Foundation of China (Grant No. 11875237).

## References

[1] Hu R, Zhu R, Wei G, Wang Z, Gu Z Y, Wanunu M and Zhao Q 2023 *Adv. Mater.* **35** 2211399
[2] Kaneko T, Okada T and Hatakeyama R 2007 *Con. Plas. Phys.* **47** 57
[3] Xie Y H, Kong Y, Soh A K and Gao H J 2007 *J. Chem. Phys.* **127** 225101
[4] Dorey A and Howorka S 2024 *Nat. Chem.* **16** 314
[5] Iqbal S M, Akin D and Bashir R 2007 *Nat. Nanotechnol.* **2** 243
[6] Haque F, Li J, Wu H C, Liang X J and Guo P 2013 *Nano Today* **8** 56
[7] Ritmejeris J, Chen X and Dekker C 2024 *Nat. Rev. Methods Primers* **3** 303
[8] Kumar H, Lansac Y, Glaser M A and Maiti P K 2011 *Soft Matter* **7** 5898
[9] Fyta M, Melchionna S and Succi S 2011 *J. Polym. Sci. Part B: Polym. Phys.* **49** 985
[10] Lin X, Chen H, Wu G, Zhao J, Zhang Y, Sha J and Si W 2024 *J. Phys. Chem. Lett.* **15** 5120
[11] Xiu P, Zhou B, Qi W, Lu H, Tu Y and Fang H 2009 *J. Am. Chem. Soc.* **131** 2840
[12] Gao H J, Kong Y, Cui D X and Ozkan C S 2003 *Nano Lett.* **3** 471
[13] Yeh I C and Hummer G 2004 *Proc. Natl. Acad. Sci. USA* **101** 12177
[14] Li J, Zhang Y, Yang J, Bi K, Ni Z, Li D and Chen Y 2013 *Phys. Rev. E* **87** 062707
[15] Mendes B B, Conniot J, Avital A, Yao D, Jiang X, Zhou X, Sharf-Pauker N, Xiao Y, Adir O, Liang H, Shi J, Schroeder A and Conde J 2022 *Nat. Rev. Methods Primers* **2** 1
[16] Wanunu M 2012 *Phys. Life Rev.* **9** 125
[17] Li J, Gong X, Lu H, Li D, Fang H and Zhou R 2007 *Proc. Natl. Acad. Sci. USA* **104** 3687
[18] Lu H, Li J, Gong X, Wan R, Zeng L and Fang H 2008 *Phys. Rev. B* **77** 174115
[19] Song C and Corry B 2009 *J. Phys. Chem. B* **113** 7642
[20] Joseph S, Mashl R J, Jakobsson E and Aluru N R 2003 *Nano Lett.* **3** 1399
[21] Geng J, Kim K, Zhang J, Escalada A, Tunuguntla R, Comolli L R, Allen F I, Shnyrova A V, Cho K R, Munoz D, Wang Y M, Grigoropoulos C P, Ajo-Franklin C M, Frolov V A and Noy A 2014 *Nature* **514** 612
[22] Liu H, He J, Tang J, Liu H, Pang P, Cao D, Krstic P, Joseph S, Lindsay S and Nuckolls C 2010 *Science* **327** 64
[23] Luan B, Zhou B, Huynh T and Zhou R 2014 *Nanoscale* **6** 11479
[24] Arai N, Koishi T and Ebisuzaki T 2021 *ACS Nano* **15** 2481
[25] Oyarzua E, Walther J H, Megaridis C M, Koumoutsakos P and Zambrano H A 2017 *ACS Nano* **11** 9997
[26] Leng J, Ying T, Guo Z, Zhang Y, Chang T, Guo W and Gao H 2022 *Carbon* **191** 175
[27] Liu C and Li Z 2010 *Phys. Rev. Lett.* **105** 174501
[28] Ostler D, Kannam S K, Daivis P J, Frascoli F and Todd B D 2017 *J. Phys. Chem. C* **121** 28158
[29] Ding C, Zhao Y and Su J 2021 *Langmuir* **37** 12318
[30] Zhang Q L, Yang R Y, Wang C L and Hu J 2022 *Phy. Rev. Fluids* **7** 114202
[31] Ostler D, Kannam S K, Frascoli F, Daivis P J and Todd B D 2019 *Langmuir* **35** 14742
[32] Wang Y, Zhao Y J and Huang J P 2011 *J. Phys. Chem. B* **115** 13275
[33] Marcotte A, Mouterde T, Niguès A, Siria A and Bocquet L 2020 *Nature Materials* **19** 1057
[34] Zhao J, Huang J Q, Wei F and Zhu J 2010 *Nano Lett.* **10** 4309
[35] Kou J, Lu H, Wu F, Fan J and Yao J 2014 *Nano Lett.* **14** 4931
[36] Zhou X Y, Kou J L, Nie X C, Wu F M, Liu Y and Lu H J 2015 *Chin. Phys. B* **24** 074702
[37] Duan W H and Wang Q 2010 *ACS Nano* **4** 2338
[38] Zhang Q L, Jiang W Z, Liu J, Miao R D and Sheng N 2013 *Phys. Rev. Lett.* **110** 254501
[39] Feng J W, Ding H M, Ren C L and Ma Y Q 2014 *Nanoscale* **6** 13606
[40] Qiu H, Shen R and Guo W 2011 *Nano Res.* **4** 284
[41] Wei M, Xu C, Zhou X and Lu H 2023 *J. Mol. Liq.* **390** 122827
[42] Zhou X, Wu F, Liu Y, Kou J and Lu H 2015 *Phys. Rev. E* **92** 053017
[43] Kang Y, Wang Q, Liu Y C, Wu T, Chen Q and Guan W J 2008 *J. Phys. Chem. B* **112** 4801
[44] Lu H J, Gong X J, Wang C L, Fang H P and Wang R Z 2008 *Chin. Phys. Lett.* **25** 1145
[45] Zhou X and Zhu F 2018 *Phys. Rev. E* **98** 032410