Rotation Motion of Designed Nano-Turbine

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Construction of nano-devices that can generate controllable unidirectional rotation is an important part of nanotechnology. Here, we design a nano-turbine composed of carbon nanotube and graphene nanoblades, which can be driven by fluid flow. Rotation motion of nano-turbine is quantitatively studied by molecular dynamics simulations on this model system. A robust linear relationship is achieved with this nano-turbine between its rotation rate and the fluid flow velocity spanning two orders of magnitude, and this linear relationship remains intact at various temperatures. More interestingly, a striking difference from its macroscopic counterpart is identified: the rotation rate is much smaller (by a factor of ~15) than that of the macroscopic turbine with the same driving flow. This discrepancy is shown to be related to the disruption of water flow at nanoscale, together with the water slippage at graphene surface and the so-called “dragging effect”. Moreover, counterintuitively, the ratio of “effective” driving flow velocity increases as the flow velocity increases, suggesting that the linear dependence on the flow velocity can be more complicated in nature. These findings may serve as a foundation for the further development of rotary nano-devices and should also be helpful for a better understanding of the biological molecular motors.

There are many nanoscopic machines in biological systems⁴–⁷. Among the most important functions of these motor proteins is to generate the rotational motion, e.g., FₐFₛ-ATPase, flagella motor. With the development of modern nanotechnology, it becomes possible to design and construct functional artificial nanoscopic devices, resembling shuttles⁸–⁹, turnstiles¹⁰, cars¹¹–¹², scissors¹³, ratchets¹⁴, and muscles¹⁵. There are many theoretical and experimental attempts to develop the nanomachine that can induce directional rotation as driven by electric or optical field¹⁶–²⁰. Even though the fluid flow is very relevant and available, the design of nano-turbine that can be driven by fluid flow is still a challenge²¹ and there are limited theoretical studies about the rotational behavior of flow-driven nano-turbine.

Here we present a designed nano-turbine constructed by a single-wall carbon nanotube (CNT) and graphene sheets. This nano-turbine can largely unidirectionally rotate as driven by a steady water flow. Despite many great progresses achieved in the development of nano-devices, the mechanism by which the nano-device works at nanoscale and the difference between the behavior of mechanical motion of a nano-device and its macroscopic analogue still largely remain elusive²². On the basis of the simulation of this designed model system, the rotation behavior of nano-turbine and the corresponding mechanism is studied in this work. We found the averaged rotation rate of the nano-turbine shows linear relationship with the flow velocity through two orders of magnitude. Compared to the macroscopic counterpart, the rotation rate of nano-turbine is much slower. Its efficiency of converting energy from fluid flow to the mechanical motion is only 6.4% of that of an ideal macroscopic counterpart. As indicated by the distribution of flow velocity, the “effective” driving flow velocity is remarkably smaller than the bulk flow velocity and the ratio can be as low as 0.15. The disruption of water flow, together with the water slippage at graphene surface and dragging effect, should be related to the much slower rotation rate. It is interesting to note that the ratio of effective driven flow velocity decreases as the flow velocity increase, suggesting that the linear relationship between rotation rate and flow velocity may be more complicated. One possible explanation of the robust linear relationship between the rotation rate and flow velocity is that the other impacts, e.g., the water slippage and dragging, may get enhanced at the same time. Meanwhile, such linear relationship remains intact at different temperatures. On the other hands, the nano-turbine is found to rotate back-and-forth in small time period (less than 1 ns), but moves forward in the long run. The ratio of the standard

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deviation to the mean value of rotation period decreases as the flow velocity increases, and the relationship between them can be fit to the reciprocal of square root function very well.

Our results exhibit the stable linear dependence of rotation rate on the flow velocity, suggesting the nano-turbine can reliably reflect the flow velocity in various environments. Such nano-turbine should also have the application in rheology measurement. As indicated by our work, the significant thermal fluctuation at the nanoscopic length scale is important to the rotation behaviors of the nano-turbine. A sufficiently large blade is necessary for the nano-turbine to be effectively driven by the fluid flow, which should be considered in the future development of fluid flow driven nano-rotors. These findings might provide some insight for the further development of rotary nano-devices and should be helpful to a better understanding of the function of biological molecular motors, e.g. $F_0F_1$-ATPase, rotary nano-devices and should be helpful to a better understanding of the function of biological molecular motors, e.g. $F_0F_1$-ATPase, flagella motor1–3, where the impact of thermal fluctuation is important to their function.

System and method

The designed nano-turbine is composed of the capped CNT and three graphene plates (Fig. 1). The (12,0) capped CNT with the length of 3.04 nm acts as the turbine axle. Three blades are made by the graphene plates covalently bonded to the CNT. The blades are parallel to the armchair direction of CNT, and the tilt angle, the angle between graphene plate and CNT axis $\beta$, is set to 58°. The dimension of graphene plate is $1.65 \times 1.33$ nm², and the radius of turbine $r = 2.1$ nm. The axle of turbine is placed along z-axis. The two fixed pole carbon atoms are shown as the golden balls. The rotation of nano-turbine is driven by the water flow along the $-z$ direction. The 2Å slab above the turbine blade is shown as the green region.

Results and discussion

Rotational motion of Nano-turbine. To achieve the directional water flow, an external force along -$z$ direction is applied to the

Figure 1 | The top view (left) and side view (right) of the designed nano-turbine placed along the $z$-axis, visualized with VMD. The two fixed pole carbon atoms are shown as the golden balls. The rotation of nano-turbine is driven by the water flow along the $-z$ direction. The 2Å slab above the turbine blade is shown as the green region.

Figure 2 | Rotation motion of nano-turbine. (a) Examples of rotation motion of nano-turbine as characterized by $\varphi$, the angle between the rotor radius vector at time $t$ with the vector at time 0. The rotation of nano-turbine is driven by the water flow of $1.82 \times 10^{-3}$ (black), $8.63 \times 10^{-3}$ (red) and $3.56 \times 10^{-2}$ nm/ps (green). (b) The rotation rate of nano-turbine, $\omega$, with respect to the average water velocity (denoted by flow velocity, $V_Z$) in 300 K. The relationship between them can be fit into a linear function very well: $\omega = -5.41 \times 10^{-3} + 0.0489 \times V_Z$ (red line).
water molecules. In this study, there are six acceleration rates have been used: $1 \times 10^{-3}$; $2 \times 10^{-3}$; $5 \times 10^{-3}$; $1 \times 10^{-2}$; $2 \times 10^{-2}$; $5 \times 10^{-2}$ nm$^2$ps$^{-2}$, corresponding to the osmotic pressure differences of 0.96, 1.92, 4.8, 9.6, 19.2, 48 Mpa (see more discussion in supplemental material). With the help of the external acceleration, the water flow along the -z direction is then generated. The averaged velocities in z-direction of bulk water are $1.82 \times 10^{-2}$, $3.63 \times 10^{-2}$, $8.63 \times 10^{-2}$, $1.8 \times 10^{-1}$, $3.56 \times 10^{-1}$, $8.9 \times 10^{-1}$ nm/ps, respectively. The averaged water velocity is proportional to the acceleration rate, in agreement with the Navier-Stokes equation (see also Fig. S2). For convenience, we use the absolute value of the average water velocity in z-direction, $V_Z$, to represent the flow velocity in the following discussion. As driven by the water flow along the -z direction the designed nano-turbine rotates largely unidirectionally in counterclockwise (CCW) direction, i.e. the nano-turbine rotates in back-and-forth in an infinitesimal time period, but moves forward in the long run. We calculated the angle between the rotor radius vector at time $t$ with the vector at time 0, $\phi(t)$, to characterize the rotational motion of turbine (Fig. 2(a)). For each flow velocity, there are at least 50 rotation periods in the simulation to achieve the reliable average value of rotation rate.

The nano-turbine rotates faster as the flow velocity increases. The rotation rate of nano-turbine, $\omega$, has an almost perfect linear relationship with the flow velocity $V_Z$ through two orders of magnitude (Fig. 2b). The fitted linear function is $\omega = -5.41 \times 10^{-1} + 0.0489 \times V_Z$, with a slope of 0.0489 nm$^{-1}$. Such linear relationship remains intact in the larger system with the size of $9 \times 9 \times 15$ nm$^3$. Moreover, the dependence of rotation rate on the flow velocity appears insensitive to the choice of thermostat method. The result obtained from the simulations using Nose-Hoover thermostat also follows the linear relationship as in the systems using the Velocity-Rescaling thermostat (Fig. S3). This linear relationship resembles the linear dependence of the rotational rate of macro-scale water turbine on the driving flow velocity. For macro-scale water turbine this linear dependence can be described in terms of the momentum exchange with water flow. In the ideal situation, the turbine rotates at such a speed that the motion of the blade is on the same pace as the water flow. Thus, the ideal rotation rate of the macro-scale turbine can be derived from the geometric transformation of the water velocity, $\omega_i = (\tan \theta/r) V$, in which $\theta$ is the tilt angle of blade, and r is the radius of turbine. In our system the value of $\tan \theta/r = 0.762$ nm$^{-1}$, which is

![Figure 3](image-url) | The distribution of average velocity of water within 2 Å water slab in the system with the flow velocity of $1.82 \times 10^{-3}$ nm/ps. (a) The fitting and the distribution of instant-average velocity of water (b) The fitting and the distribution of time-average velocity of water with the window size of 1 (black), 10 (red) and 50 ps (green).

![Figure 4](image-url) | The fitting and the distribution of time-average velocity of water within a smaller 2Å-slab with the window size of 1 (black) 10 (red) and 50 ps (green). The size of this water slab is $0.8 \times 0.66$ nm$^2$, one fourth of the blade size of the nano-turbine in this work.

![Figure 5](image-url) | The distribution of $V_{Z,local}$ along the z-axis in the system with the flow velocity of $8.63 \times 10^{-2}$ nm/ps. In the region above the turbine blade, the $V_{Z,local}$ decrease as the water get close to the blade (region 1); in the corresponding region of the blade (region 2) it increases sharply; then the $V_{Z,local}$ relaxes to 0.0069 nm/ps in region3 before it finally converges to the bulk value (region 4).
much larger than the slope from the above linear fit for the nano-turbine. Here we introduce a slowing factor $a$ to characterize this discrepancy, with $a = \omega_0/\omega_i = 0.064$. The rotation rate of the nano-turbine appears to be much slower ($\approx 15\times$) than its macroscale analogue. As indicated by the macroscopic turbine flow meter, the discrepancy of actual rotation speed from the ideal rotation speed is less than 8\%\textsuperscript{29}.

Mechanisms of the Rotational Behavior of Nano-turbine. It is well accepted that the thermal noise is profound in the microscopic environment. The extent of thermal motion of water can be orders of magnitude larger than the actual flow velocity in our systems. In order to address the question on how the designed nano-turbine can still rotate largely unidirectionally when the flow velocity is relatively small, we first calculated the instant-average velocity of water by averaging the velocity of water molecules within a slab, with the size of the slab chosen as the blade size and the thickness of the slab 2 Å. As depicted in Fig. 1, the 2-Å slab is immediately above turbine blade, with same tilt angle as the blade. The instant-average water velocity is highly fluctuating even after averaging. Here we examine the system with the flow velocity of $1.82 \times 10^{-3}$ nm/ps as an example. The width of the distribution of instant-average water velocity is $5.93 \times 10^{-2}$ nm/ps, which is still more than one order of magnitude larger than the flow velocity (Fig. 3a). The direction of water flow flips frequently. The probability of having instant-average velocity of water along $-z$ direction is only 53%, barely larger than the probability of being along the opposite $+z$ direction. However the nano-turbine rotates largely unidirectionally (according to a net force from $-z$ direction water flow), in counterclockwise direction rather than in highly random manner. The amplitude of the

![Figure 6](https://www.nature.com/scientificreports/4:5846.png)
fluctuation of rotation angle (the extent of rotating backward) keeps less than 10 degree in all the systems (Fig. S4), even though the frequency of rotating backward is large when flow velocity is small (the frequency can be more than 140 ns⁻¹ when the flow velocity is 1.82 × 10⁻² nm/ps). The relationship of the frequency of net rotation and the flow velocity can be fitted to a linear function very well (see Fig. S5). In summary, the relative fluctuations of the rotational motion are considerably smaller than the thermal fluctuation of the water velocity.

We further calculated the averaged velocity of water molecules within the 2 Å thick slab over a period of time, denoted by time-averaged water velocity. As one can expect, the fluctuation of time-averaged water velocity becomes smaller than the instant-average velocity of water. As the averaging window size increases, the fluctuation of time-averaged water velocity gets sharper. Thus, the probability of having velocity of water molecules is more than 140 ns⁻¹ when the flow velocity is 1.82 × 10⁻² nm/ps. The relationship of the frequency of net rotation and the flow velocity can be fitted to a linear function very well (see Fig. S5). In summary, the relative fluctuations of the rotational motion are considerably smaller than the thermal fluctuation of the water velocity.

As the flow velocity increases, the extent of rotation of the nano-turbine decreases. As the flow velocity increases, the extent of rotation of the nano-turbine decreases. The rotation of even smaller nano-turbines may not be effectively driven by the fluid flow. The choice of the size of the nano-turbine, especially the blade size, thus is crucial to achieve a reliable performance of nano-turbines.

To further study the driving mechanism of rotation of the nano-turbine, we analyzed the velocity distribution of the water molecules in the vicinity region of nano-turbine (the cylinder region along the nano-turbine axis). Here we use the system with the flow velocity of 8.63 × 10⁻⁵ nm/ps as an example. As shown in Fig. 5 the water velocity ($V_{z,local}$) is remarkably different along the z-axis, while such dramatically fluctuating velocity distribution will be almost completely smoothed out in macroscopic turbine flow meter. The distribution of $V_{z,local}$ can be divided into four regions. In the region above the turbine blade (region 1), the water velocity declines as the water molecules get close to the blade. And the average velocity of water directly above the blade ($V_{z,local}$ at z = 57 Å), i.e. the effective driving flow velocity, is 2.98 × 10⁻⁴ nm/ps, only 34% of the bulk value. In the region corresponding to the blade (region 2) the average water velocity grows sharply to 9 × 10⁻⁴ nm/ps. And then the average water velocity relaxes to 6.9 × 10⁻⁴ nm/ps in the region of 48 Å > z > 37 Å (region 3) before it finally converges to the bulk average value of 8.63 × 10⁻⁵ nm/ps (region 4).

The decrement of $V_{z,local}$ in the region 1 can be related to the much slower rotation rate of the nano-turbine. Again, we use the ratio of effective driving flow velocity to the bulk water velocity to characterize the effect of the disruption of water flow above the blade. Now consider the flow velocity and the broad distribution of individual water velocities within a 2-Å water slab, there is a considerable portion of water molecules whose velocities are larger than the velocity of the rotation of nano-turbine. Thus these water molecules bounce back from the upper surface of turbine blade, and disturb the water flow in the region above. The orientation of water molecules may be affected as well. On the other hand, the water velocity sharply increases in region 2. The acceleration partly comes from the momentum exchange with the bulk water which has larger average velocity. However, the change in region 2 is more dramatic than in region 4 which is also due to the momentum exchange with the bulk water. Therefore, there should be another source for the acceleration. As discussed above, the distribution of velocity of individual water molecules is very broad, and there should be also a considerable portion of water molecules whose velocities are smaller than the velocity of the rotation of the nano-turbine or even moving along the opposite direction. Thus, these water molecules under the blade are pushed forward by the blades, and that also contributes to the acceleration in region 2. In other words, the rotation motion of nano-turbine is dragged by the water molecules below the blade, i.e. the dragging effect on the rotation motion. Besides, water exhibit considerable slippage at graphene surface, therefore, these water slippage also contribute to the much slower rotation motion. It should be noted that the slippage of water molecules can also be attributed to the hydrophobicity of graphene blade. Hence, the rotation rate of nanoturbine (i.e. the efficiency of converting energy) should be affected by the degree of hydrophobicity of graphene blade.

As suggested by the dramatically fluctuating velocity distribution, the much slower rotation rate of the nano-turbine can be attributed to several effects, including water flow disruption and the dragging effect, together with the water slippage at graphene surface. Consequently, the rotation rate of the nano-turbine is much slower than the macroscopic counterpart, where the rotation motion is close to the ideal case driven by the homogeneous water flow, and can be described with a simple geometric transformation of water flow velocity. The discrepancy of actual rotation speed from the ideal rotation speed is less than 8%. And there should be an upper limit of efficiency for the nano-device converting the energy from fluid flow energy to the rotational motion.

Similar distributions of the velocities of water molecules in the vicinity region of nano-turbine are observed in the systems with different flow velocities (Fig. 6). The effective driving flow velocities (the average velocity of water directly above the blade) of all six systems are 2.91 × 10⁻⁴, 1.05 × 10⁻⁴, 2.98 × 10⁻⁴, 8.46 × 10⁻², 1.96 × 10⁻², 5.34 × 10⁻² nm/ps, respectively. Unlike the constant slowing factor $\alpha = 0.064$, the ratio of effective driving velocity to bulk value increases from 0.16 to 0.6 as the flow velocity increases (Fig. 7).
The disruption of the water flow in region 1 becomes less significant when the rotation rate increases. While the linear relationship between rotation rate and flow velocity remains intact, implying that the other effects such as the dragging and water slippage may become more profound as the rotation rate increases. On the basis of this robust linear relationship, the slowing factor \( \alpha \) can then serve as the characteristic of the nano-turbine. It should be noted that the estimate of the efficiency of energy conversion is based on the idealized free-standing nano-turbine, the efficiency would become even smaller if it is loaded with a resistive coupler. And there should be an upper limit of efficiency for a given nano-device converting the energy from fluid flow energy to the rotational motion. These findings may serve as a foundation for the further development of nano-turbine to improve the efficiency of energy conversion.

Figure 8 | The fluctuation of rotation period is characterized by the ratio of the standard deviation to the average value of rotation period. The relationship between them can be fit to the reciprocal of square root function, \( R = 0.15 \times V_z^{-0.5} \) (red curve).

Conclusions

In this work, we designed a nano-turbine that can rotate largely unidirectionally as driven by the directional water flow. Several features of the rotation motion of nano-turbine are observed on the basis of the simulation of this model system. The rotation rate increases linearly with the flow velocity through two orders of magnitude. Comparing to the macroscopic counterpart, the rotation rate of the nano-turbine is much smaller. As indicated by the dramatically fluctuating velocity distribution, much slower rotation rate can be attributed to several effects including the flow disruption, dragging effect, together with the slippage on graphene surface. Moreover, the ratio of effective driving flow velocity increases as the flow velocity increases, indicating the reduced overall disruption effect. It suggests that the other effects such as water slippage and dragging get profound concomitantly to ensure the stable linear relationship. Beside the much slower rotation motion, the nano-turbine is found to rotate back-and-forth in small time period (less than 1 ns) even though it moves forward in the long run. The fluctuation of the rotation period decreases as the average water velocity increases. The relationship between the extent of fluctuation and the average water velocity can be fit to a reciprocal of square root very well. Our results suggest the significance of thermal fluctuation on the rotary behavior of the nano-turbine. So the choice of a sufficiently large blade is important for the performance of the nano-turbine. These findings might provide some insight to the further development of rotary nano-devices and should help to achieve a better understanding of the function of biological molecular motors. We also studied the rotation motion of nano-turbine in different temperatures (i.e. 300 K and 360 K). The linear relationship remains intact at different temperature. In this way, this nano-turbine can not only harvest
Figure 10 | The relationship among the flow velocity, driving force and rotation rate in 300 K and 360 K. (a) The dependence of the rotation rate on the driving force $F_z$. With the same driving force, the nano-turbine rotates faster due to the smaller water viscosity at 360 K. (b) the relationship between the driving force and the flow velocity. Under the same flow velocity, the exerting force of water is smaller at 360 K because of smaller viscosity.
