Electronic Supplementary Material (ESI) for Nanoscale.


# Supplementary information

## Actuation Mechanism of a Nanoscale Drilling Rig Based on Nested Carbon Nanotubes

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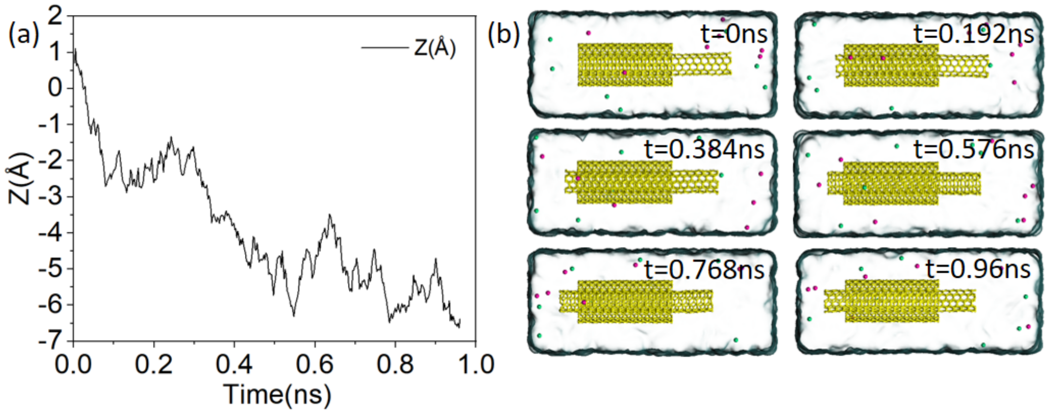


Figure S1. MD simulation of nanoscale drilling rig without charge. (a) The displacement curve of the inner wall CNT1 of the nanoscale drilling rig along the Z-axis direction over time. (b) The microstructure sequence during the operation of a non-charged nanoscale drilling rig. The yellow color in the figure represents carbon nanotubes. The inner carbon nanotube is an armchair shaped carbon nanotube with a size of (5,5) and a height of 50 angstroms. The outer carbon nanotube is an armchair shaped carbon nanotube with a size of (10,10) and a height of 30 angstroms.

This experiment can prove that the displacement of carbon nanotubes along the negative Z-axis is not caused by the addition of ribbon nanoelectrodes, but by the asymmetry of the nanoscale drilling rig itself.

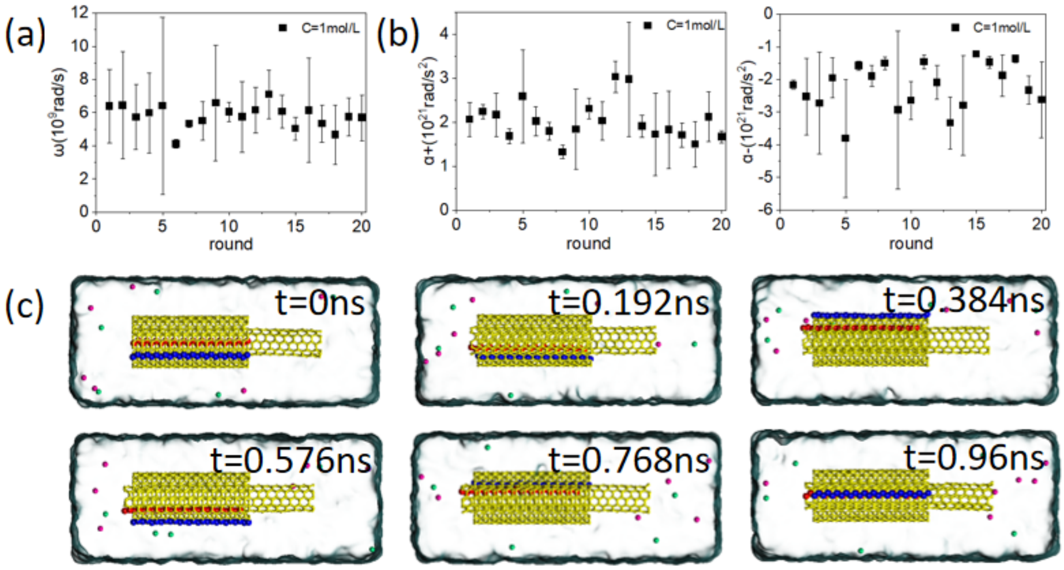


Figure S2. Simulation of the rotation process of a nanoscale drilling rig under a concentration of 1mol/L. (T=295K, q=0.1e, f=20.83ns$^{-1}$, r=3.39 Å) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

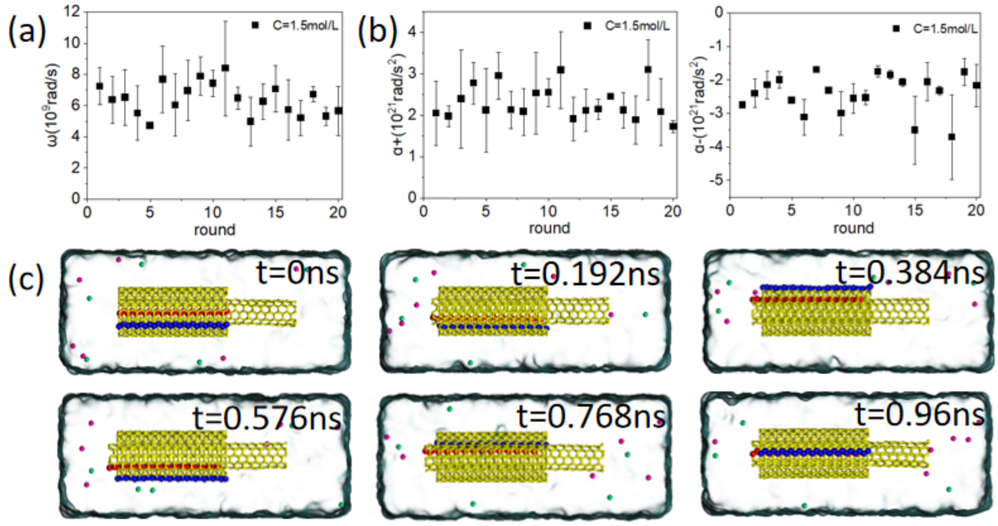


Figure S3. Simulation of the rotation process of a nanoscale drilling rig under a concentration of 1.5mol/L. (T=295K, q=0.1e, f=20.83ns$^{-1}$, r=3.39 Å) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

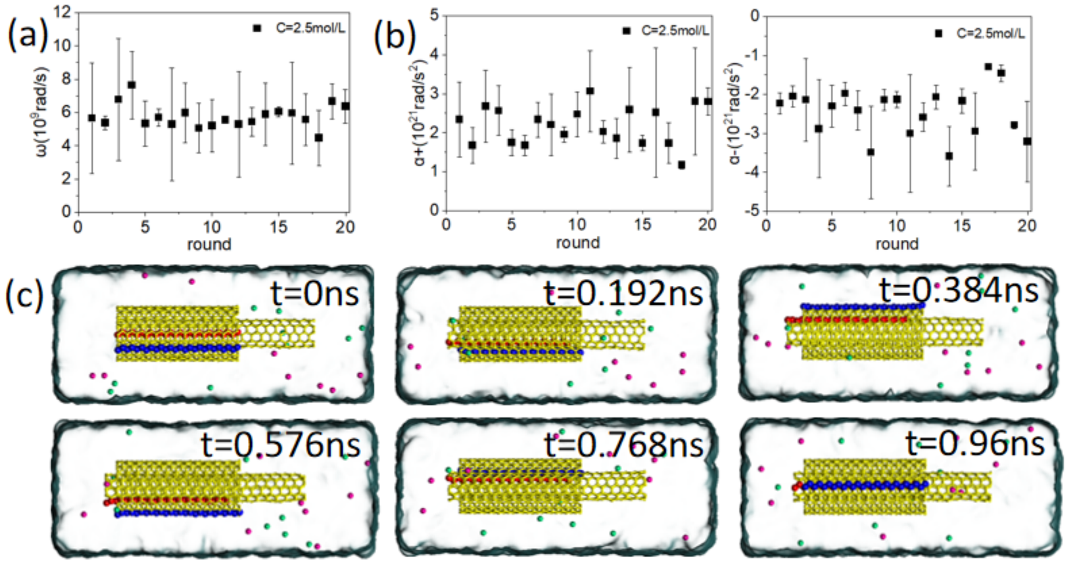


Figure S4. Simulation of the rotation process of a nanoscale drilling rig under a concentration of 2.5mol/L. (T=295K, q=0.1e, f=20.83ns$^{-1}$, r=3.39 Å) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

From Figures S2-S4, it can be seen that as the ion concentration in the nanoscale drilling rig system increases, the angular velocity and positive and negative angular acceleration of the nanoscale drilling rig during each round fluctuate around a fixed value. This proves that changes in ion concentration do not cause changes in the rotation of nanoscale drilling rigs, which is in line with our expected results.

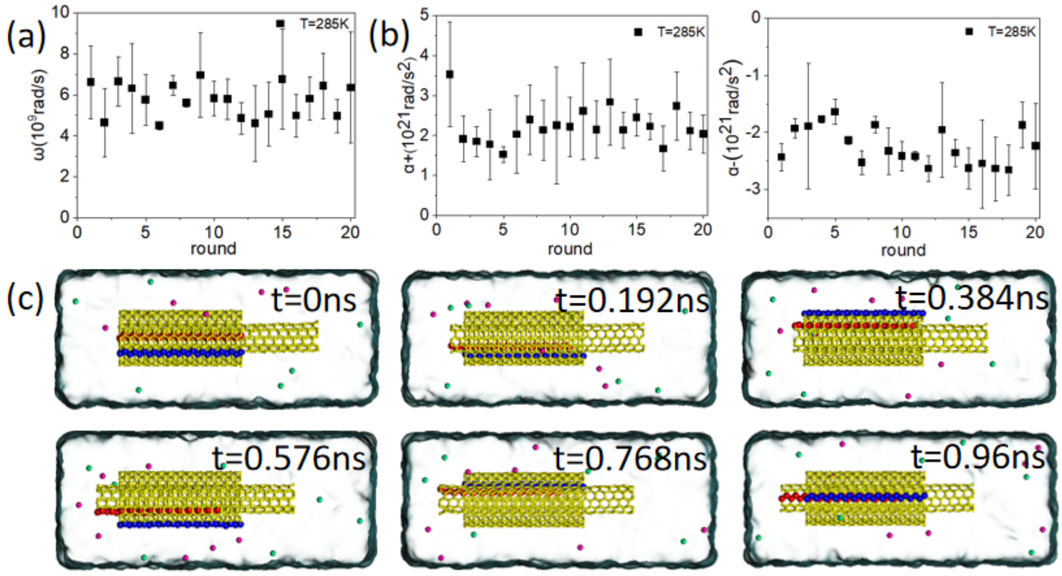


Figure S5. Simulation of the rotation process of a nanoscale drilling rig under a temperature of 285K. (C=2mol/L, q=0.1e, f=20.83ns$^{-1}$, r=3.39 Å) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

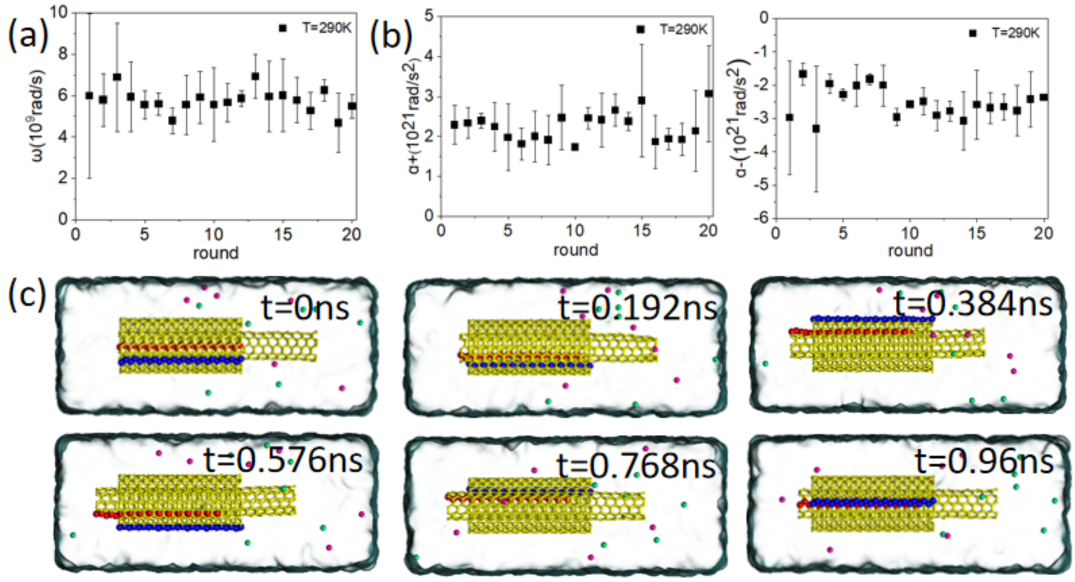


Figure S6. Simulation of the rotation process of a nanoscale drilling rig under a temperature of 290K. (C=2mol/L, q=0.1e, f=20.83ns$^{-1}$, r=3.39 Å) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

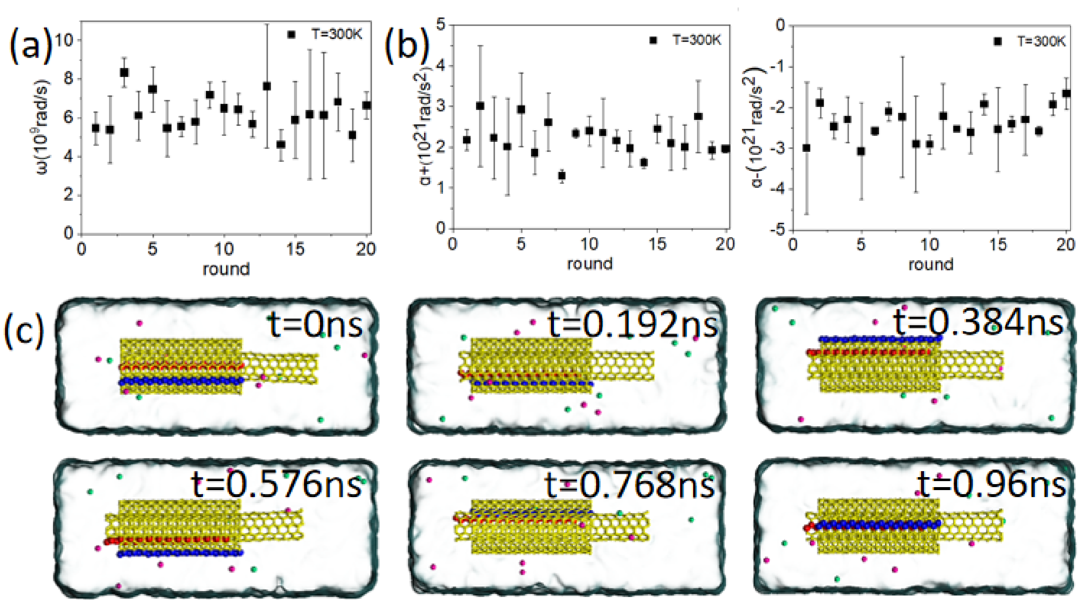


Figure S7. Simulation of the rotation process of a nanoscale drilling rig under a temperature of 300K. (C=2mol/L, q=0.1e, f=20.83ns$^{-1}$, r=3.39 Å) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

From Figures S5-S7, it can be seen that as the temperature in the nanoscale drilling rig system increases, the angular velocity and positive and negative angular acceleration of the nanoscale drilling rig during each round fluctuate around a fixed value. This proves that changes in temperature do not cause changes in the rotation of nanoscale drilling rigs, which is in line with our expected results.

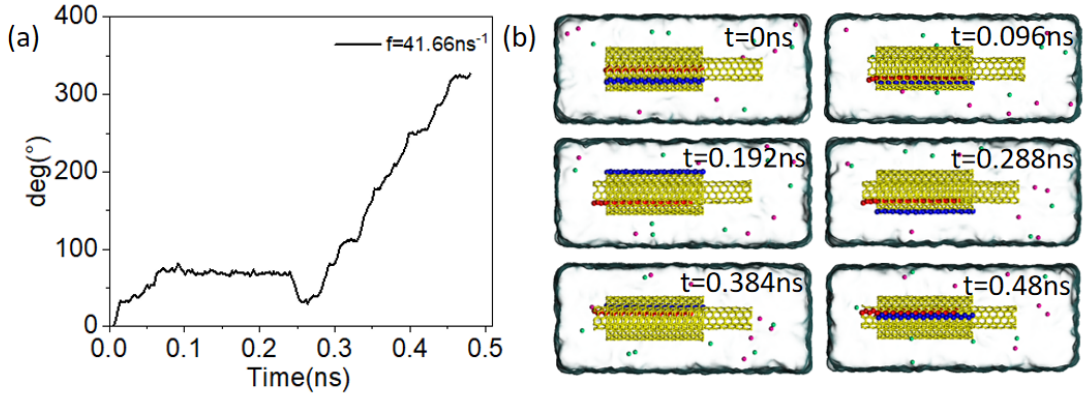


Figure S8. Simulation of the rotation process of nanoscale drilling rigs under the condition of charge switching frequency of 41.66ns$^{-1}$. (T=295K, C=2mol/L, q=0.1e, r=3.39 Å) (a) The variation of the rotation angle of a nanoscale drilling rig with the rotation period. Among them, the rotation lasted for two cycles. (b) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has a negative charge on top.

From the graph, it can be seen that when the charge switching frequency is too fast, the nanoscale drilling rig exhibits a phenomenon of stopping or even reversing. This is due to the fact that the rotation speed of the inner carbon nanotubes cannot keep up with the switching speed of the electrodes on the outer carbon nanotubes. Therefore, when using a nanoscale drilling rig, it is necessary to control the switching frequency of the outer wall charge to match the rotational speed of the inner wall.

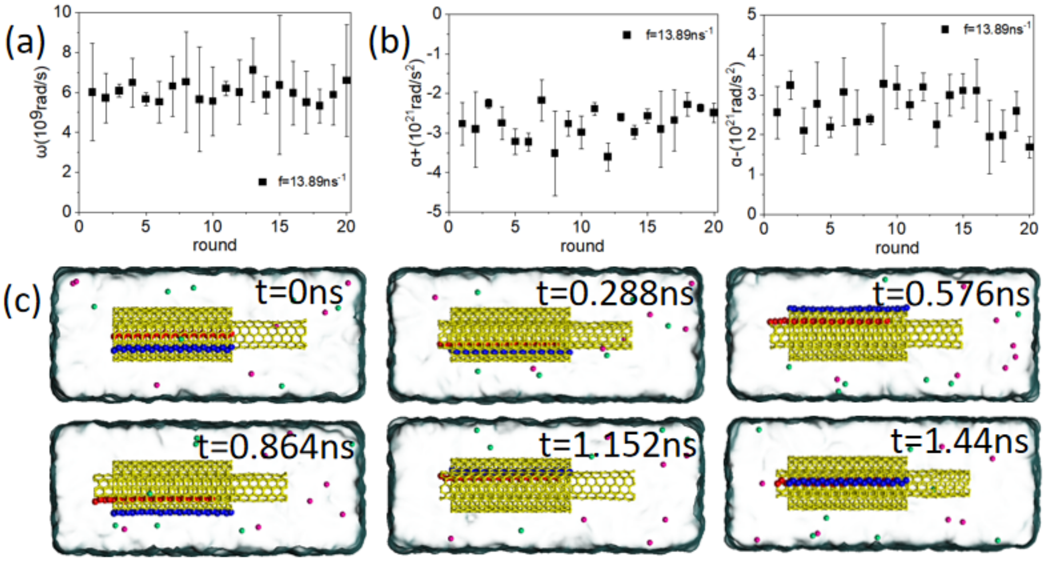


Figure S9. Simulation of the rotation process of nanoscale drilling rigs under the condition of charge switching frequency of 13.89ns$^{-1}$. (T=295K, C=2mol/L, q=0.1e, r=3.39 Å) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

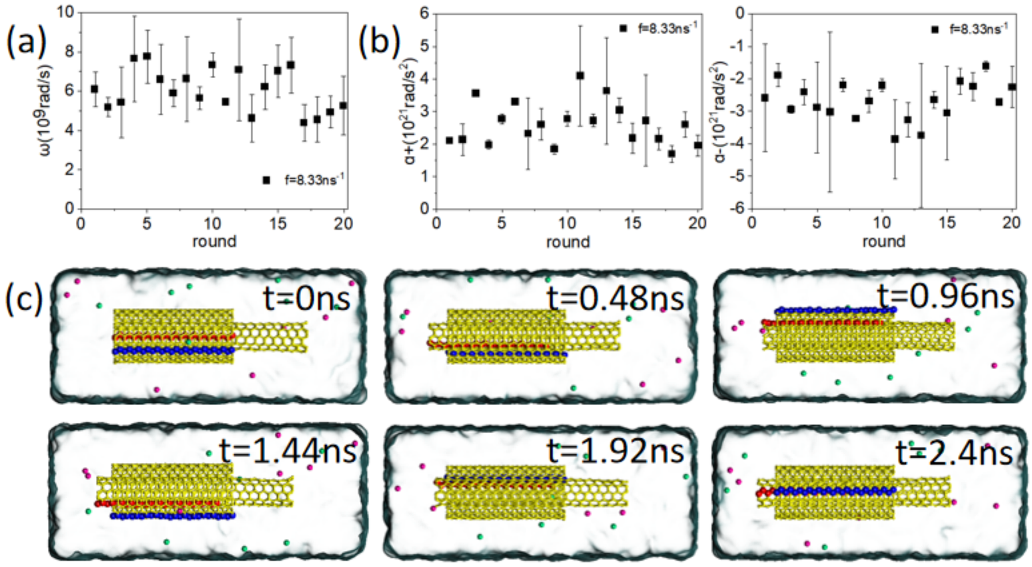


Figure S10. Simulation of the rotation process of nanoscale drilling rigs under the condition of charge switching frequency of 8.33ns$^{-1}$. (T=295K, C=2mol/L, q=0.1e, r=3.39 Å) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

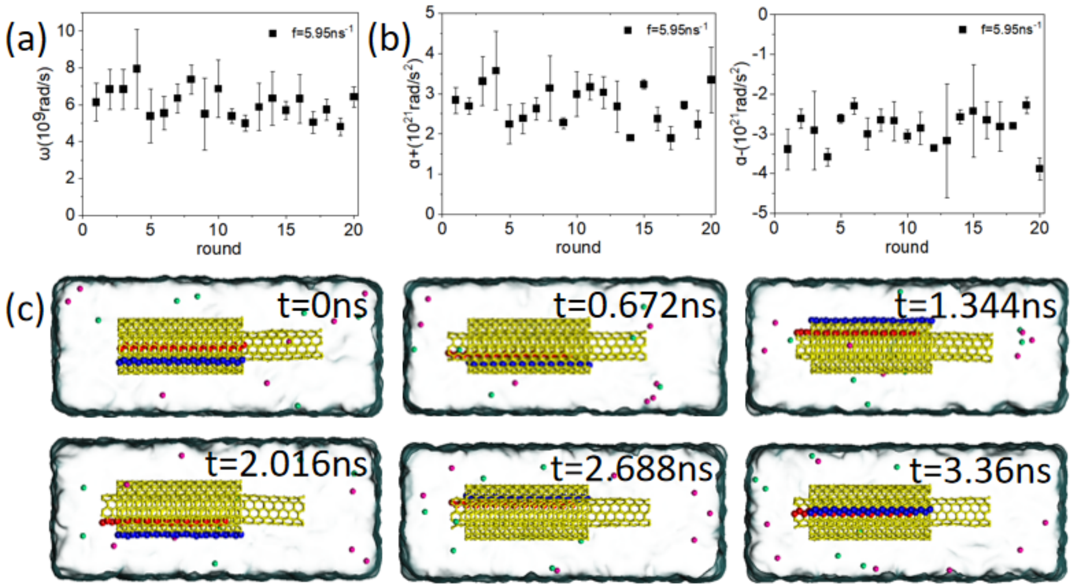


Figure S11. Simulation of the rotation process of nanoscale drilling rigs under the condition of charge switching frequency of 5.95ns$^{-1}$. (T=295K, C=2mol/L, q=0.1e, r=3.39 Å) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

From Figures S9-S11, it can be seen that as the charge switching frequency in the nanoscale drilling rig system decreases, the angular velocity and positive and negative angular acceleration of the nanoscale drilling rig during each round fluctuate around a fixed value. This proves that changes in charge switching frequency do not cause changes in the rotation of nanoscale drilling rigs, which is in line with our expected results.

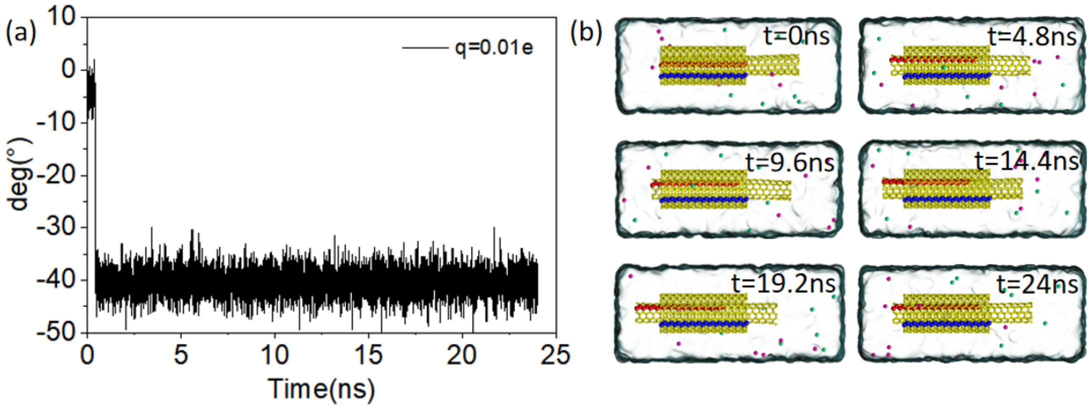


Figure S12. Simulation of the rotation process of a nanoscale drilling rig with a single atom carrying a charge of 0.01e on a strip-shaped nanoelectrode. (T=295K, C=2mol/L, r=3.39 Å) (a) The variation of the rotation angle of a nanoscale drilling rig with the rotation period. Among them, the rotation lasted for two cycles. (b) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has a negative charge on top.

From the graph, it can be seen that when a single atom of the nanoelectrode carries a charge of 0.01e, the nanoscale drilling rig still cannot rotate normally after a long period of time. Because at this distance, the charge force acting on the inner layer of carbon nanotubes is smaller than the van der Waals force between the inner and outer walls. Therefore, in certain special situations where a nanoscale drilling rig needs to slow down, we do not recommend setting the charged amount of the nanoelectrode too low, otherwise it will cause the nanoscale drilling rig to malfunction.

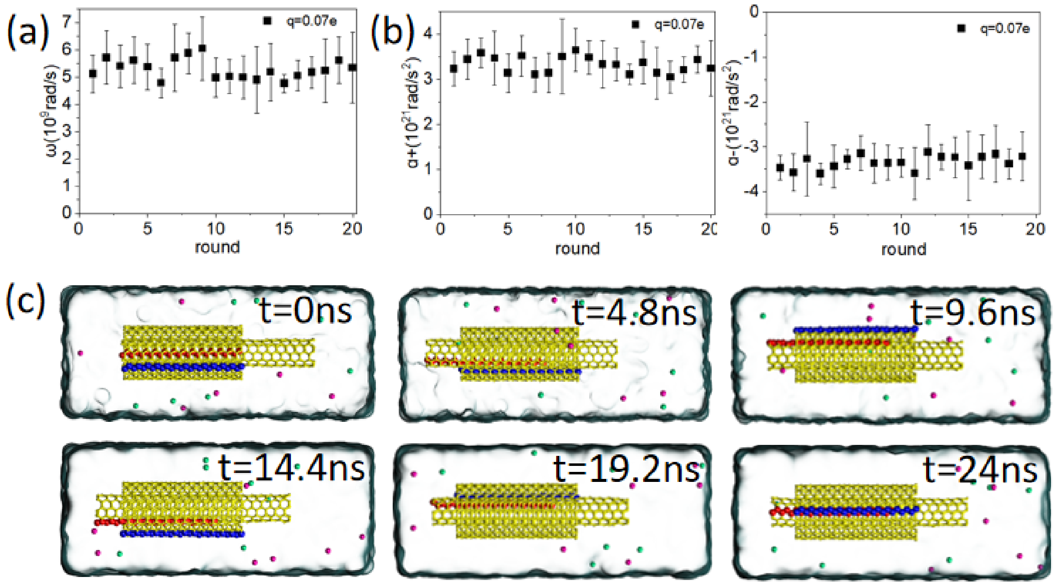


Figure S13. Simulation of the rotation process of a nanoscale drilling rig with a single atom carrying a charge of 0.07e on a strip-shaped nanoelectrode. (T=295K, C=2mol/L, r=3.39 Å)(a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

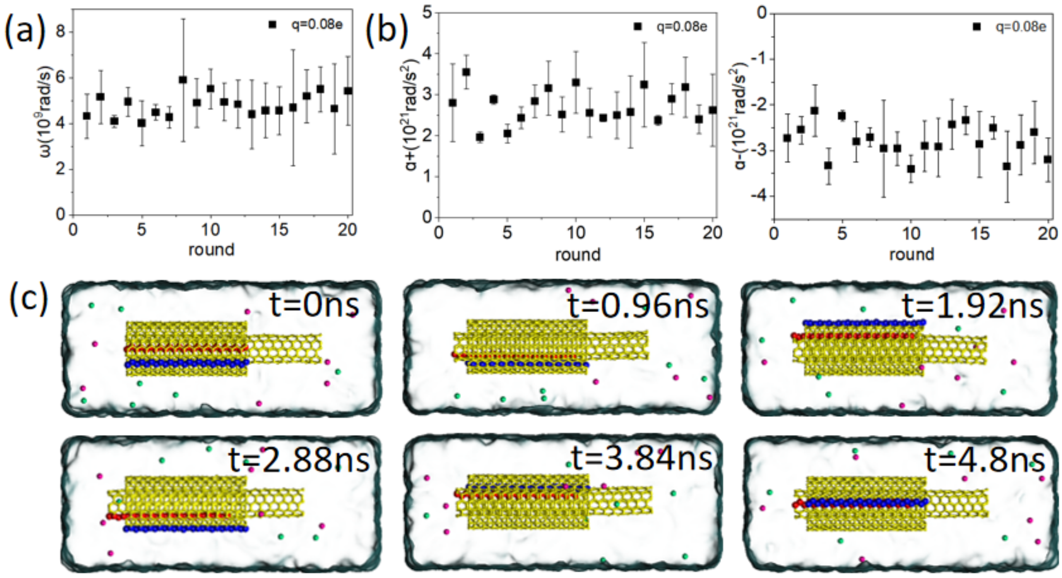


Figure S14. Simulation of the rotation process of a nanoscale drilling rig with a single atom carrying a charge of 0.08e on a strip-shaped nanoelectrode. (T=295K, C=2mol/L, r=3.39 Å)(a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

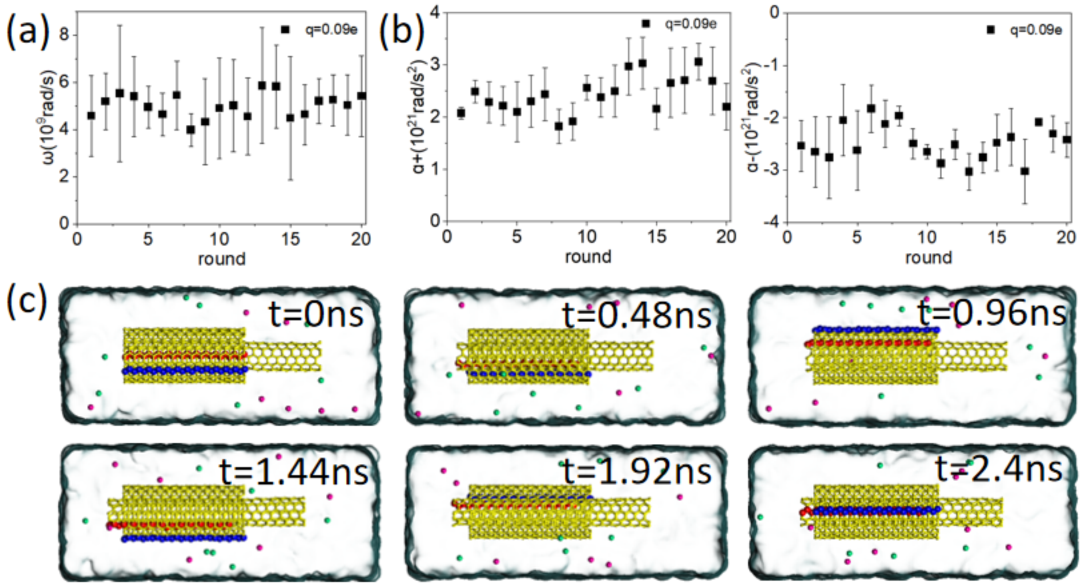


Figure S15. Simulation of the rotation process of a nanoscale drilling rig with a single atom carrying a charge of 0.09e on a strip-shaped nanoelectrode. (T=295K, C=2mol/L, r=3.39 Å)(a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrodes with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

From Figures S13-S15, it can be seen that as the amount of charge carried by a single atom in the striped nanoelectrode increases, the angular velocity and positive and negative angular acceleration values of the nanoscale drilling rig during each cycle also increase accordingly. This is because the electrostatic force between the two nanoelectrodes is improved, so the nanoscale drilling rig has more sufficient power, resulting in faster rotation.

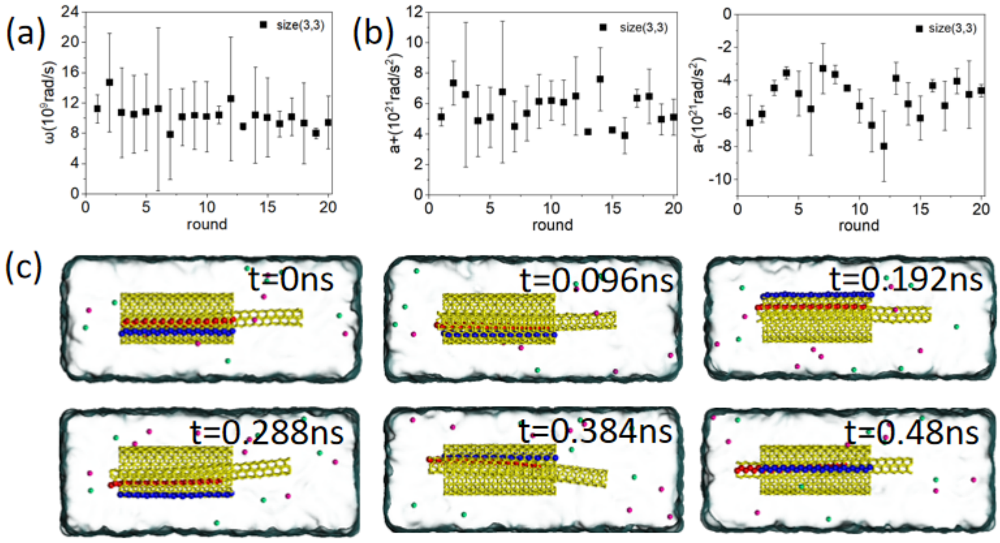


Figure S16. Simulation of the rotation process of a nanoscale drilling rig when the size of the inner layer of carbon nanotubes is (3,3). (T=295K, C=2mol/L, q=0.01e) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

During the rotation process, the inner layer of carbon nanotubes showed bending. This is because the force applied to carbon nanotubes through strip shaped nanoelectrodes is uneven. When the diameter of the inner layer of carbon nanotubes in nanoscale drilling rigs decreases, they are more susceptible to external forces, resulting in deformation.

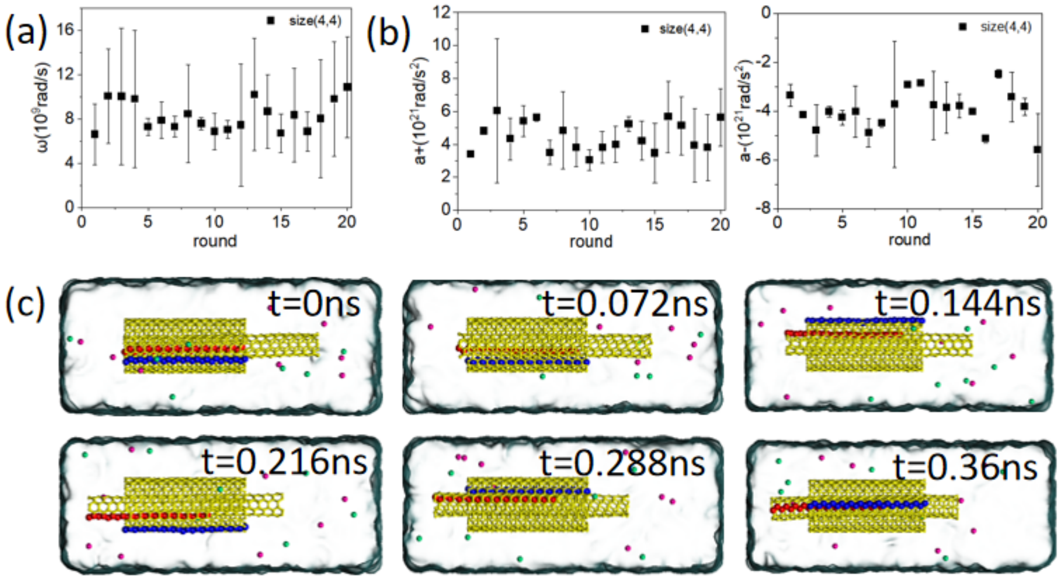


Figure S17. Simulation of the rotation process of a nanoscale drilling rig when the size of the inner layer of carbon nanotubes is (4,4). (T=295K, C=2mol/L, q=0.01e) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

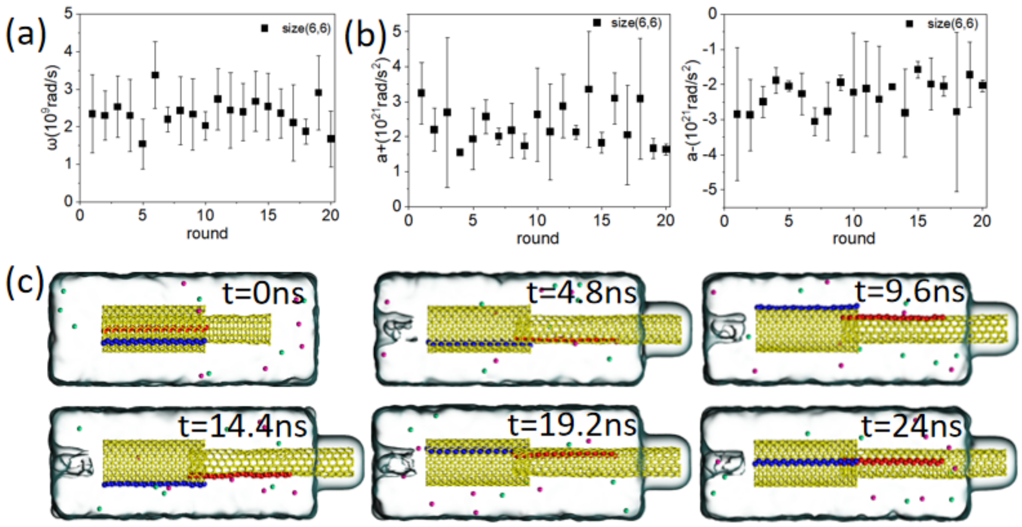


Figure S18. Simulation of the rotation process of a nanoscale drilling rig when the size of the inner layer of carbon nanotubes is (6,6). (T=295K, C=2mol/L, q=0.01e) (a) The variation of rotational angular velocity of a nanoscale drilling rig with rotation period. The simulation lasts for a total of 20 periods. Among them, the error bar represents the standard error. (b) The variation of positive and negative angular acceleration of nanoscale drilling rig rotation with rotation period. (c) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrode with positive charges on top. The blue color represents the outer nanoelectrode, which has negative charges on top.

From Figures S16-S18, it can be seen that as the diameter of the inner layer carbon nanotubes of the nanoscale drilling rig increases, the angular velocity and positive and negative angular acceleration of the nanoscale drilling rig during each period will correspondingly decrease. This is because the spacing between the inner and outer layers of carbon nanotubes on the nanoscale drilling rig has decreased at this time. The increase in van der Waals force is greater than the increase in electrostatic force, resulting in a slower rotation of the nanoscale drilling rig. In addition, we found that in a nanoscale drilling rig with a carbon nanotube inner size of (6,6), the length of the inner layer carbon nanotubes protruding is much longer than in other situations, which will be explained in detail later.

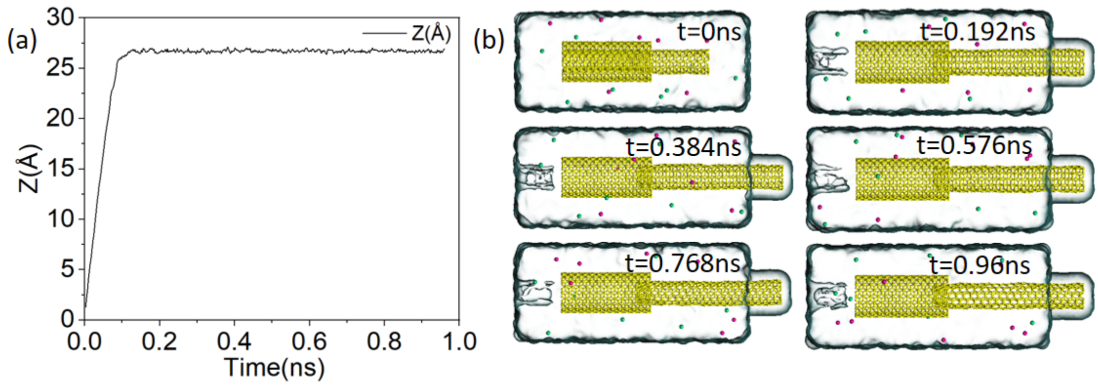


Figure S19. Simulation of the rotation process of a nanoscale drilling rig when the size of the inner layer of carbon nanotubes is (6,6). (T=295K, C=2mol/L) (a) The displacement of the inner wall of a nanoscale drilling rig along the Z-axis direction over time. (b) The microstructure sequence during the rotation process of nanoscale drilling rigs. Among them, yellow represents carbon nanotubes.

From Figures S18-S19, it can be seen that when no charge is added to the nanoelectrode, the inner layer carbon nanotubes of the nanoscale drilling rig still exhibit a significant extension along the Z-axis direction. This is because this phenomenon is not caused by electrostatic forces, but by van der Waals forces. When the distance between the inner and outer walls of a nanoscale drilling rig is too close, the van der Waals force is greater and exhibits repulsive force. Therefore, the inner carbon nanotubes of the nanoscale drilling rig are pushed out under the action of repulsion, causing a longer distance of displacement.

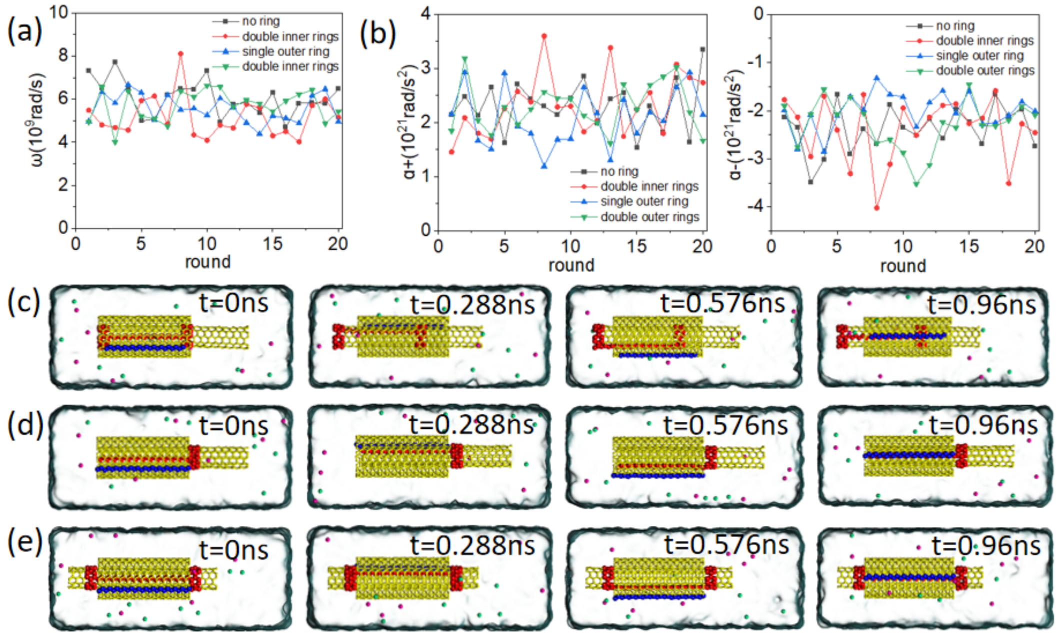


Figure S20. Simulation of nanoscale drilling machines with annular electrodes carried at different positions. (a) The variation of the rotational angular velocity of inner carbon nanotubes with different nanoscale drilling rigs. (T=295K, C=2mol/L, f=20.83ns$^{-1}$, q=0.1e) (b) The variation of positive and negative angular accelerations of inner carbon nanotubes rotation with different nanoscale drilling rigs. (c) Microscopic simulation sequence of a nanoscale drilling rig with two annular nanoelectrodes installed inside the outer layer of carbon nanotubes. Among them, yellow represents carbon nanotubes. The red color indicates the inner layer of nanoelectrodes with positive charges on top. The blue color represents the outer nanoelectrode, which has a negative charge on top. (d) Microscopic simulation sequence of a nanoscale drilling rig with an annular electrode installed outside the outer layer of carbon nanotubes. (e) Microscopic simulation sequence of a nanoscale drilling rig with two annular electrodes installed outside the outer layer of carbon nanotubes.

As shown in the figure, whether without the addition of circular nanoelectrodes or when the position of the circular nanoelectrodes is changed, the angular velocity, positive and negative angular acceleration, and microstructure sequence of the nanoscale drilling rig during each cycle all fluctuate within a certain range. This further confirms the conclusion that the double electron layer will not affect the rotation of nanoscale drilling machines.