Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

A Controllable Nanoscale Telescopic Arm Designed by Encoding the Nested Multi-walled Carbon Nanotubes

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Figure S1 shows that the charged inner wall exhibits a slight protrusion at its initial point of contact, which may be attributed to the attractive forces arising from water polarization.

Figures S2-S4 show that by increasing the magnitude of the electric field, a greater electric field force can be obtained. This results in a reduction in the fluctuation of the displacement curve of the inner wall, leading to enhanced stability of the system. Furthermore, the switching time for the electric field is reduced, allowing the inner wall to respond more quickly for the applied electric field.

Figure S5 shows that using an alternating electric field would have a significant impact on the operating status of the telescopic arm.

Figures S6-S8 show that as the radius difference between the inner and outer carbon tubes increases, the van der Waals (vdW) resistance decreases during the forward stroke, ultimately resulting in a more stable and rapid movement. Conversely, during the backward stroke, the smaller traction of vdW force leads to a reduction in velocity and the displacement curve oscillates more obviously.

Figures S9-S10 show the local ion concentration distributions in different conditions. For example, as the carbon nanotube is positively charged and the charge density increases, its ability to adsorb chloride ions becomes enhanced, resulting in a more stable electric double layer.

Figure S11 shows the ion mobility distribution along *z*-axis *versus* distance from the central axis of the single-walled carbon nanotube.

Figure S12 shows the ion concentration distribution *versus* distance from the central axis of the single-walled carbon nanotube.

Figures S13-S14 show MD simulations of manipulation of multi-walled carbon nanotube telescopic arm hovering at length of $\frac{1}{2}l$ when extending.

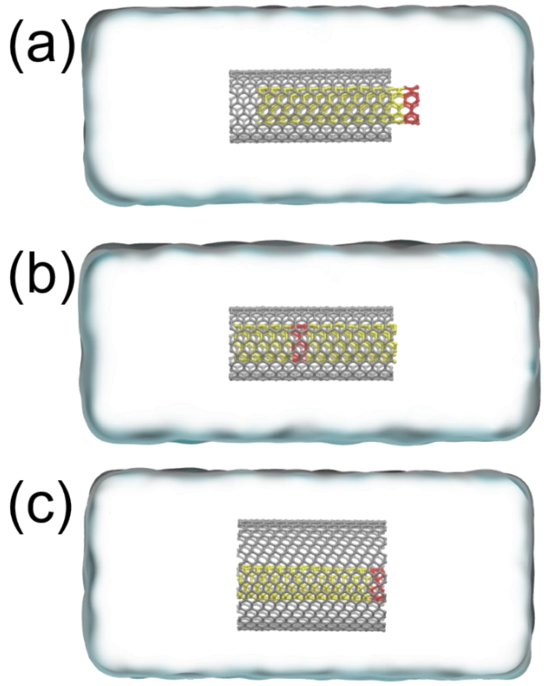

Figure S1. Initial displacement of inner carbon nanotube under different state of contact with TIP3 water molecules. (a) One end of the inner carbon nanotube is charged. Due to the electrostatic force of the nanoring, the water molecules are polarized and attract the inner wall to extend. When the entire nanoring is in contact with water molecules, the forces are balanced in all directions. (b) The nanoring located in the middle of the inner carbon nanotube is charged. Since the inner wall is separated from the water molecules by the outer wall, water molecules are not polarized due to the larger gap. Thus, the inner carbon nanotube was not attracted by the water molecules and keep in place. (c) A double wall carbon nanotube with an outer wall of larger diameter and one end of the inner wall is charged. The gap between the inner wall and outer wall allows water molecules to enter. Since the water molecules are in contact with entire charged nanorings at the beginning, the forces were balanced and the inner wall did not extend.

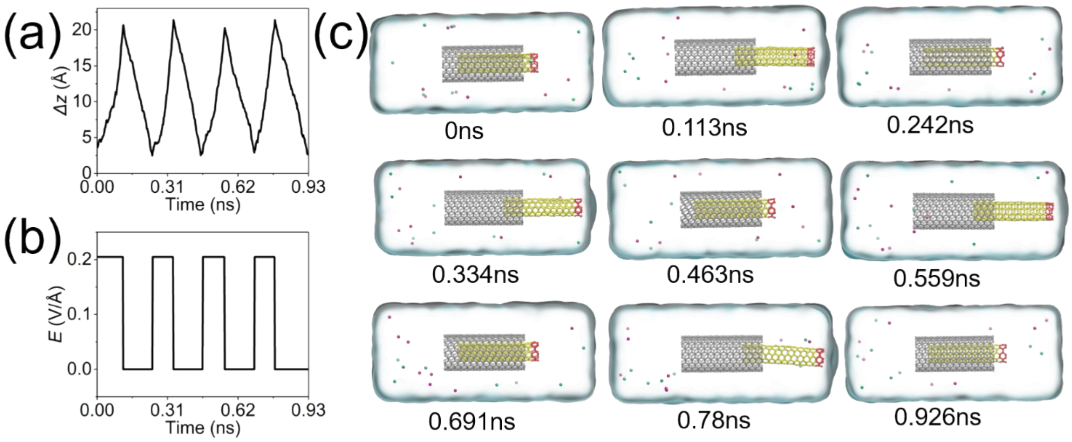

Figure S2. MD simulation of the reciprocating motion of the double wall carbon nanotube telescopic arm under E=0.2V/Å. (a) The displacement curve of the CNT_1 mass center versus time, which includes 4 times of reciprocating motion. (b) The control strategy of the applied electric field to realize the manipulation of the double wall carbon nanotube telescopic arm. When strength of the applied electric field is set as 0.2V/Å, the arm will extend and when the strength of the applied electric field is set as 0, the arm will retract. (c) Four cycles of reciprocating motion of the telescopic arm corresponding to curve in Figure 2a. The bit code of the nanoring is '001' which means the $ring_2$ and $ring_3$ are uncharged and the $ring_1$ is positively charged. Thus $ring_{2,3}$ are hidden for clarity.

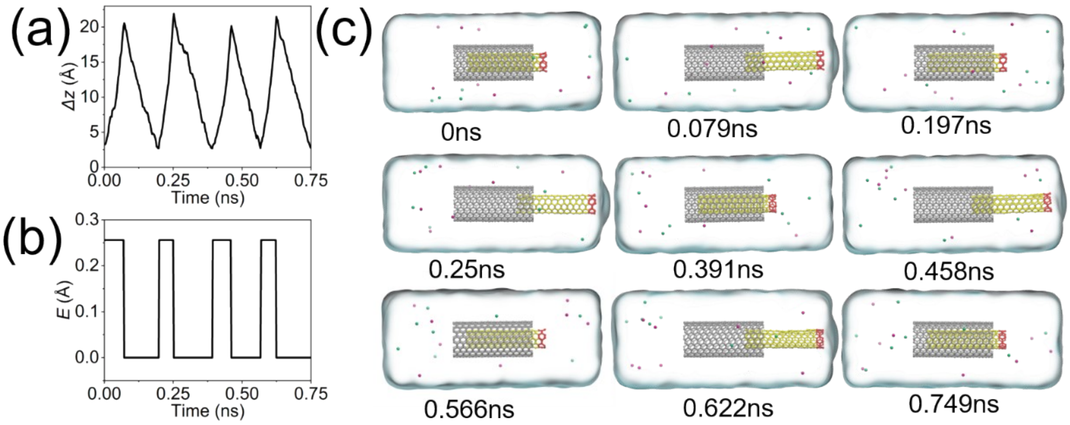

Figure S3. MD simulation of the reciprocating motion of the double wall carbon nanotube telescopic arm under E=0.26V/Å. (a) The displacement curve of the CNT_1 mass center versus time, which includes 4 times of reciprocating motion. (b) The control strategy of the applied electric field to realize the manipulation of the double wall carbon nanotube telescopic arm. When strength of the applied electric field is set as 0.26V/Å, the arm will extend and when the strength of the applied electric field is set as 0, the arm will retract. (c) Four cycles of reciprocating motion of the telescopic arm corresponding to curve in Figure 2a. The bit code of the nanoring is '001' which means the $ring_2$ and $ring_3$ are uncharged and the $ring_1$ is positively charged. Thus $ring_{2,3}$ are hidden for clarity.

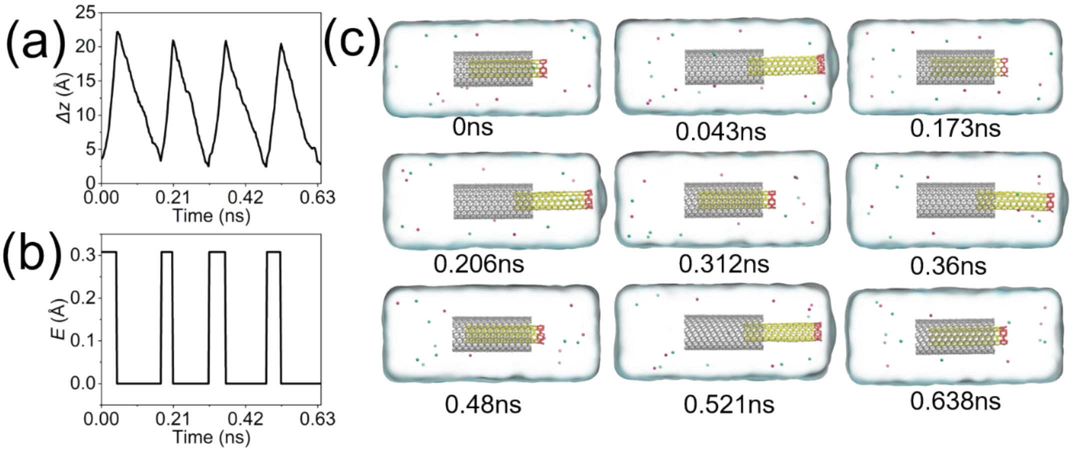

Figure S4. MD simulation of the reciprocating motion of the double wall carbon nanotube telescopic arm under E=0.3V/Å. (a) The displacement curve of the CNT_1 mass center versus time, which includes 4 times of reciprocating motion. (b) The control strategy of the applied electric field to realize the manipulation of the double wall carbon nanotube telescopic arm. When strength of the applied electric field is set as 0.3V/Å, the arm will extend and when the strength of the applied electric field is set as 0, the arm will retract. (c) Four cycles of reciprocating motion of the telescopic arm corresponding to curve in Figure 2a. The bit code of the nanoring is '001' which means the $ring_2$ and $ring_3$ are uncharged and the $ring_1$ is positively charged. Thus $ring_{2,\ 3}$ are hidden for clarity.

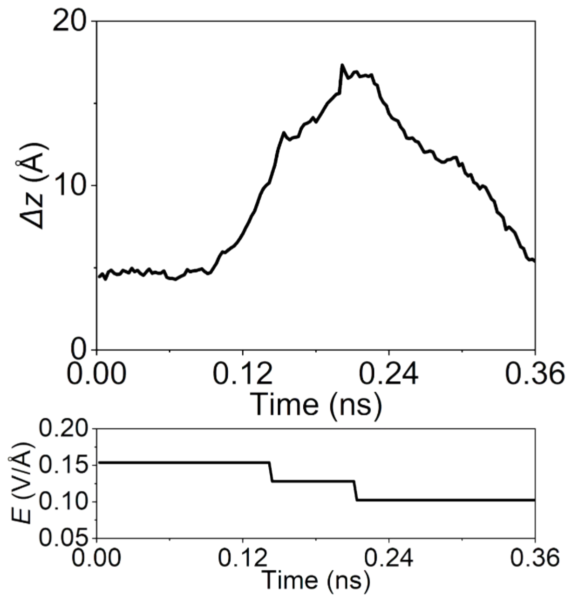

Figure S5. MD simulation of the pushing-out motion of the double-walled carbon nanotube telescopic arm under an alternating *E*. An electric field of 0.16 V/Å was initially applied, then the electric field was decreased to 0.13 V/Å, resulting in a reduction in the slope of the displacement trace of inner CNT, indicating a corresponding decrease in the speed of the inner wall. Subsequently, as the electric field was further decreased to 0.1 V/Å, interestingly the inner wall was gradually retracted due to insufficient electric field force compared to the vdW force.

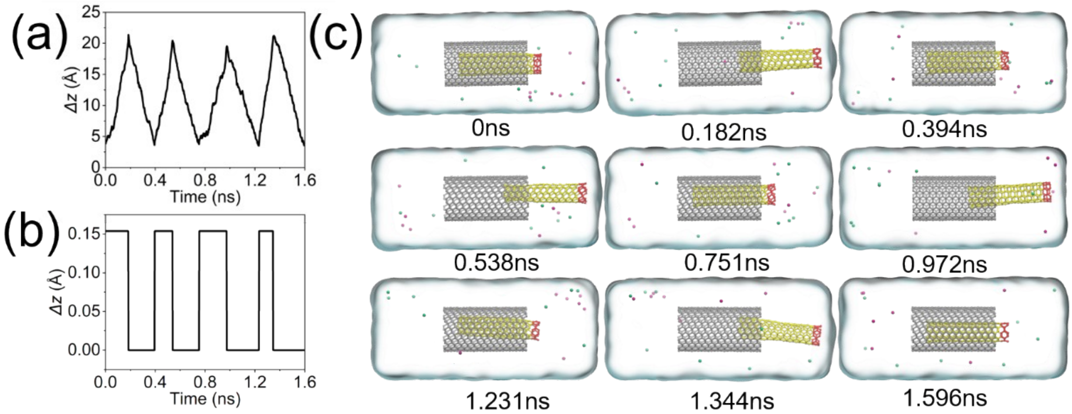

Figure S6. MD simulation of the reciprocating motion of the double wall carbon nanotube telescopic arm when the diameter of the outer wall is set to 16.27Å. (a) The displacement curve of the CNT_1 mass center versus time, which includes 4 times of reciprocating motion. (b) The control strategy of the applied electric field to realize the manipulation of the double wall carbon nanotube telescopic arm. When strength of the applied electric field is set as 0.15V/Å, the arm will extend and when the strength of the applied electric field is set as 0, the arm will retract. (c) Four cycles of reciprocating motion of the telescopic arm corresponding to curve in Figure 2a. The bit code of the nanoring is '001' which means the $ring_2$ and $ring_3$ are uncharged and the $ring_1$ is positively charged. Thus $ring_{2}$, $_{3}$ are hidden for clarity.

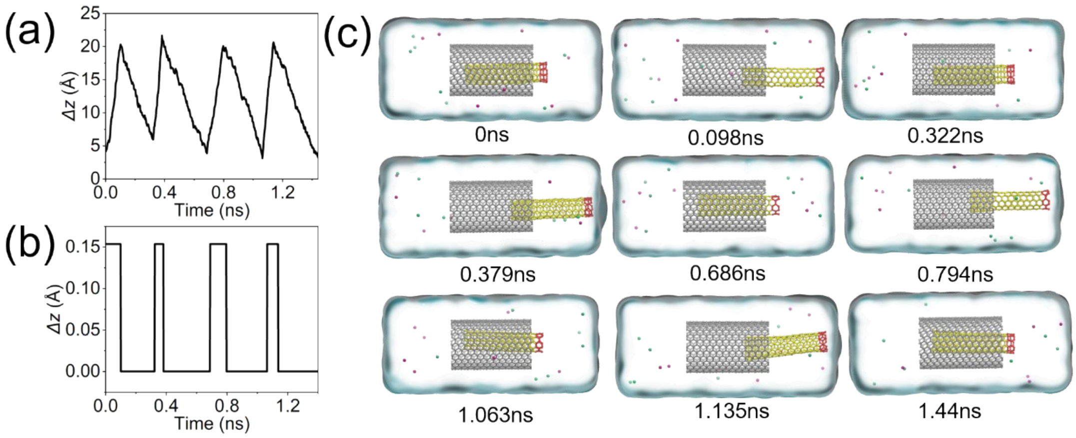

Figure S7. MD simulation of the reciprocating motion of the double wall carbon nanotube telescopic arm when the diameter of the outer wall is set to 18.98Å. (a) The displacement curve of the CNT_1 mass center versus time, which includes 4 times of reciprocating motion. (b) The control strategy of the applied electric field to realize the manipulation of the double wall carbon nanotube telescopic arm. When strength of the applied electric field is set as 0.15V/Å, the arm will extend and when the strength of the applied electric field is set as 0, the arm will retract. (c) Four cycles of reciprocating motion of the telescopic arm corresponding to curve in Figure 2a. The bit code of the nanoring is '001' which means the $ring_2$ and $ring_3$ are uncharged and the $ring_1$ is positively charged. Thus $ring_{2,\ 3}$ are hidden for clarity.

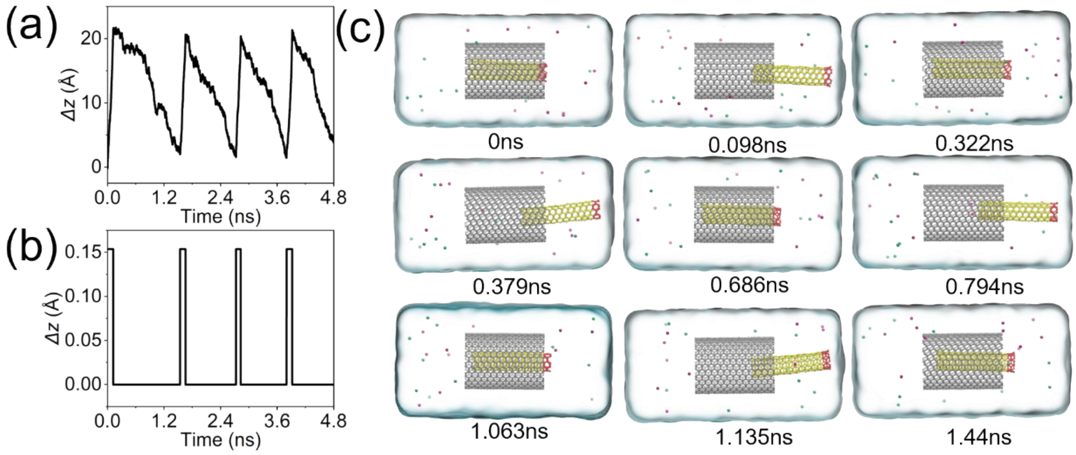

Figure S8. MD simulation of the reciprocating motion of the double wall carbon nanotube telescopic arm when the diameter of the outer wall is set to 21.7Å. (a) The displacement curve of the CNT_1 mass center versus time, which includes 4 times of reciprocating motion. (b) The control strategy of the applied electric field to realize the manipulation of the double wall carbon nanotube telescopic arm. When strength of the applied electric field is set as 0.15V/Å, the arm will extend and when the strength of the applied electric field is set as 0, the arm will retract. (c) Four cycles of reciprocating motion of the telescopic arm corresponding to curve in Figure 2a. The bit code of the nanoring is '001' which means the $ring_2$ and $ring_3$ are uncharged and the $ring_1$ is positively charged. Thus $ring_{2,3}$ are hidden for clarity.

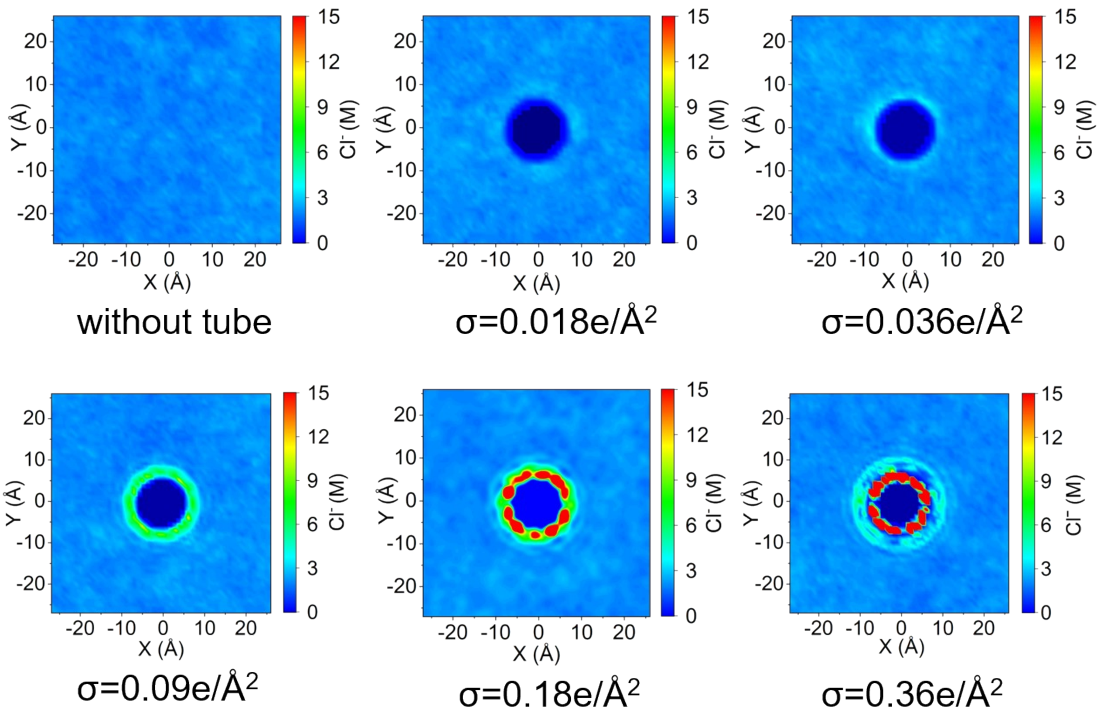

Figure S9. Local ion concentration distribution of Cl^- on the *x*-*y* cross section.

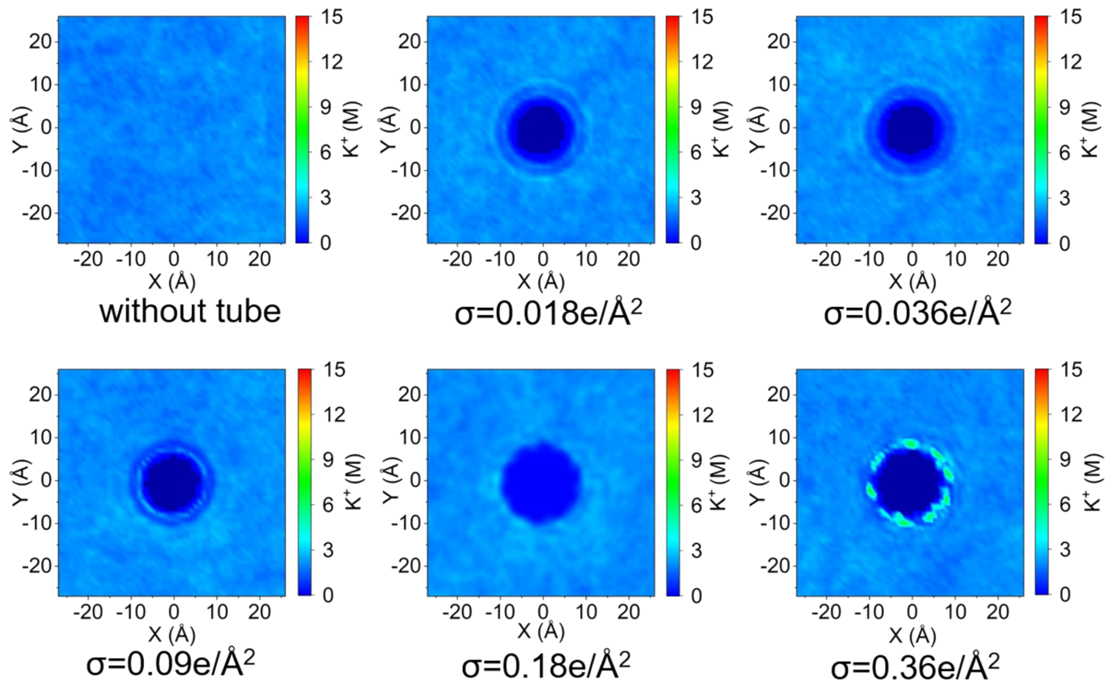

Figure S10. Local ion concentration distribution of K^+ on the *x*-*y* cross section.

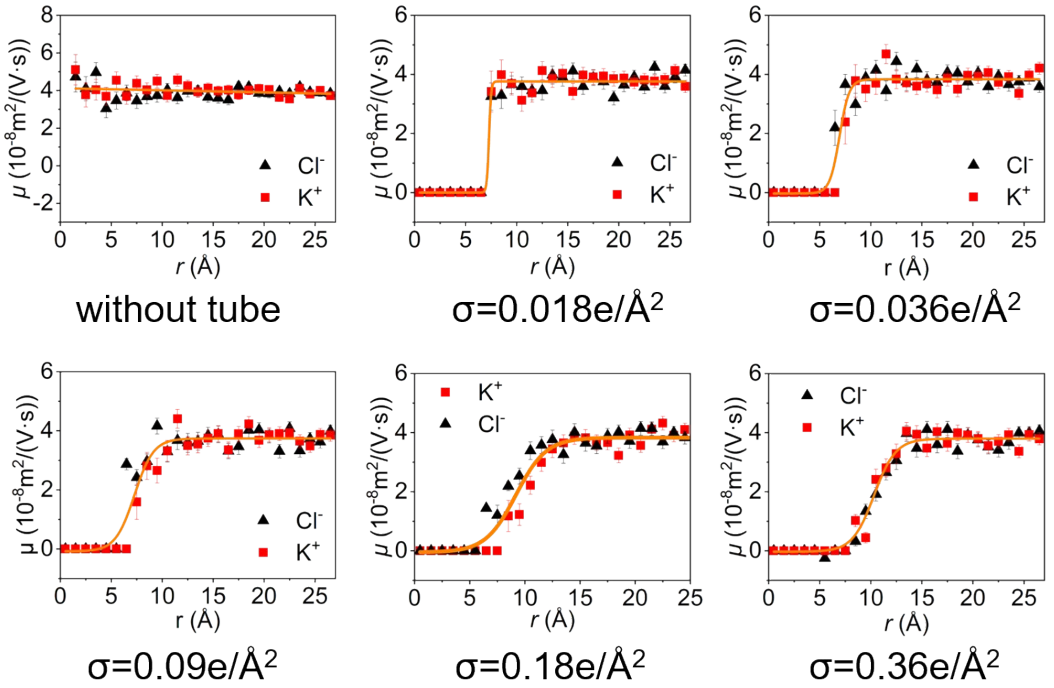

Figure S11. The ion mobility along z-axis versus distance from the central axis of the single wall carbon nanotube. The data point of the potassium ions concentration is shown as red square and the chloride ions concentration is shown as black triangle. The fitted curve of the ion mobility is shown in orange.

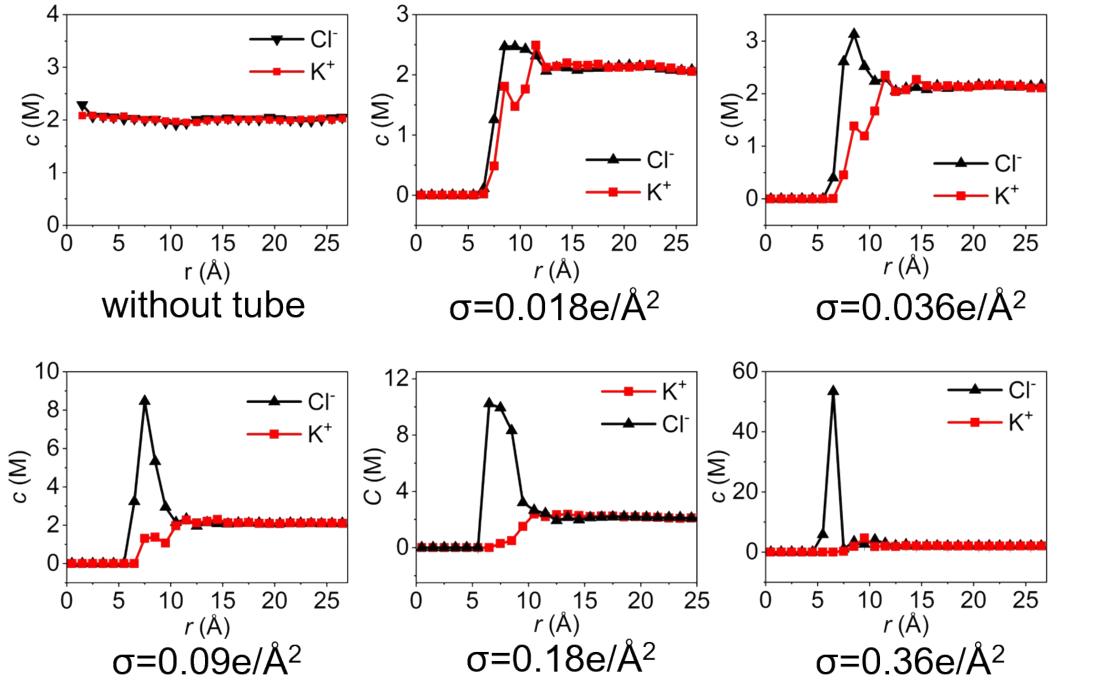

Figure S12. The ion concentration versus distance from the central axis of the single-wall carbon nanotube. The data point of the potassium ions concentration is shown as red square linked by red line and the chloride ions concentration is shown as black triangle linked by black line.

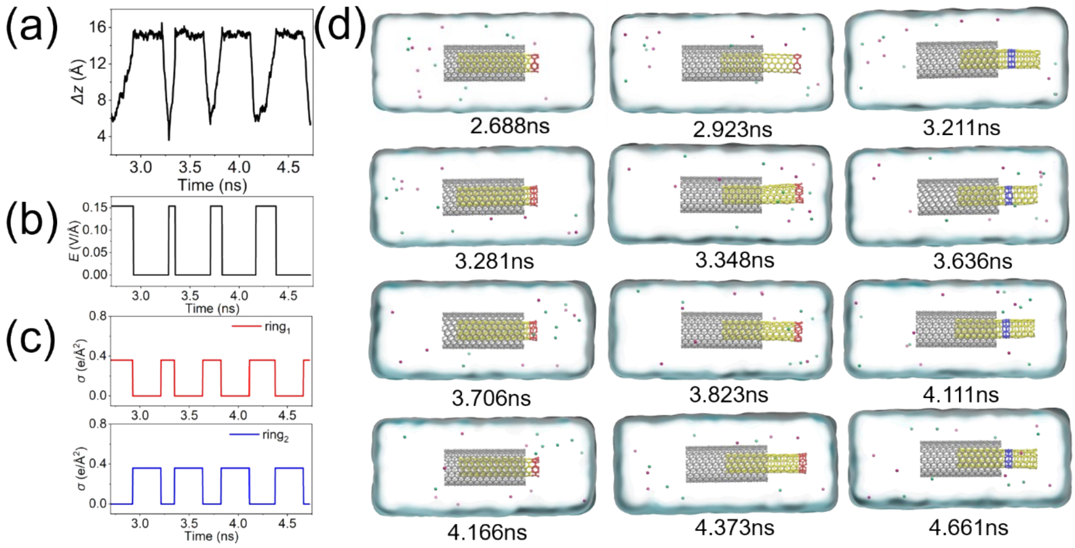

Figure S13. MD simulation of manipulation of DWCNT telescopic arm hovering at length of $\frac{1}{2}l$ when extending. (a) The displacement trace of the CNT_1 mass center versus time, which includes 4 times of reciprocating motion. (b) The control strategy of the applied electric field to realize the manipulation of the DWCNT telescopic arm. (c) The control strategy of the nanorings charge density to realize the manipulation of the DWCNT telescopic arm. (d) Four cycles of reciprocation motion of the telescopic arm corresponding to the first trapezoidal curve in Figure S12a.

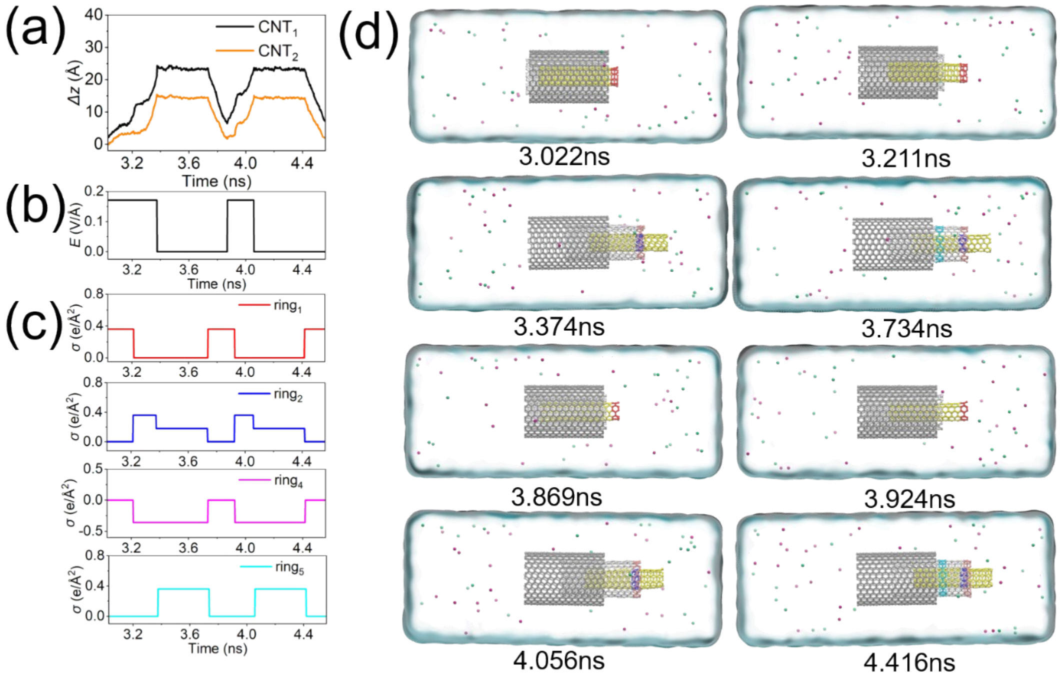

Figure S14. MD simulation of manipulation of three wall carbon nanotube telescopic arm hovering at length of $\frac{1}{2}l$ when extending. (a) The displacement trace of the CNT_1 and CNT_2 mass center versus time, which includes 2 times of reciprocating motion. (b) The control strategy of the applied electric field to realize the manipulation of three wall carbon nanotube telescopic arm. (c) The control strategy of the nanorings charge density to realize the manipulation of three wall carbon nanotube telescopic arm. (d) Two cycles of reciprocation motion of the telescopic arm corresponding to the first trapezoidal curve in Figure S13a.