Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Pumping of water by rotating chiral carbon nanotube

Jia-wei Feng,[a] Hong-ming Ding,[a] Chun-lai Ren[a] and Yu-qiang Ma*[ab]

[a] *National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China.*
[b] *Center for Soft Condensed Matter Physics and Interdisciplinary Research, Soochow University, Suzhou 215006, China.*
* *E-mail: myqiang@nju.edu.cn*

1 STRUCTURE OF WATER INSIDE THE CNT

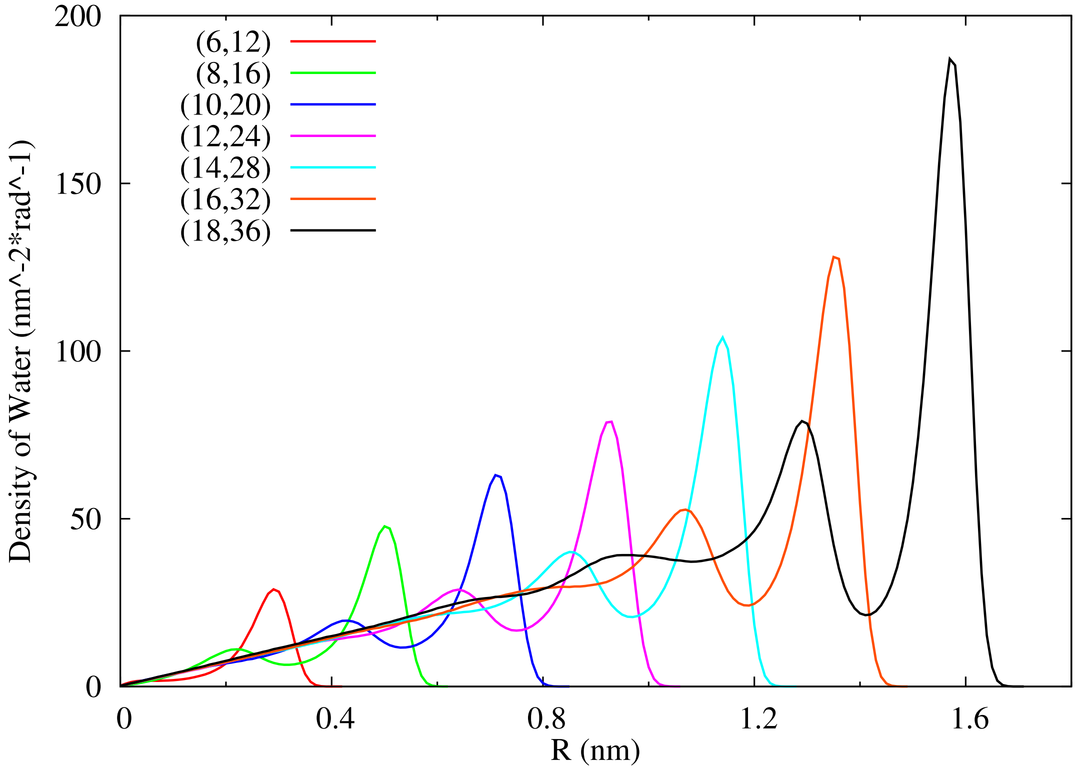

Fig. S 1 Density profiles of water inside all kinds of CNTs.

2 AXIS DISTRIBUTION FUNCTION (ADF) OF WATER INSIDE THE CNT

The ADF of water $ADF(z)$ is defined as $\int_0^L ADF(z)\pi R^2 dz = N - 1 \approx N$, where N is the number of water molecules between z=0 to z=L.

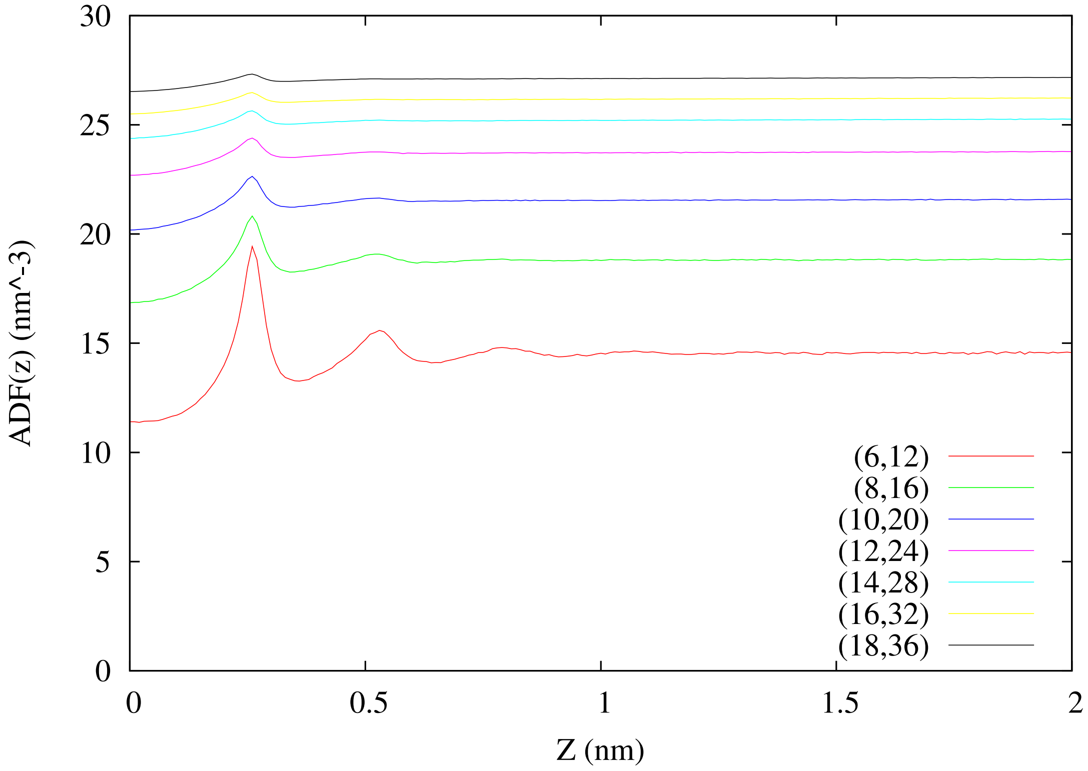

Fig. S 2 ADF of water inside the CNT.

3 POTENTIAL ENERGY LANDSCAPES BETWEEN CNT AND WATER MOLECULE

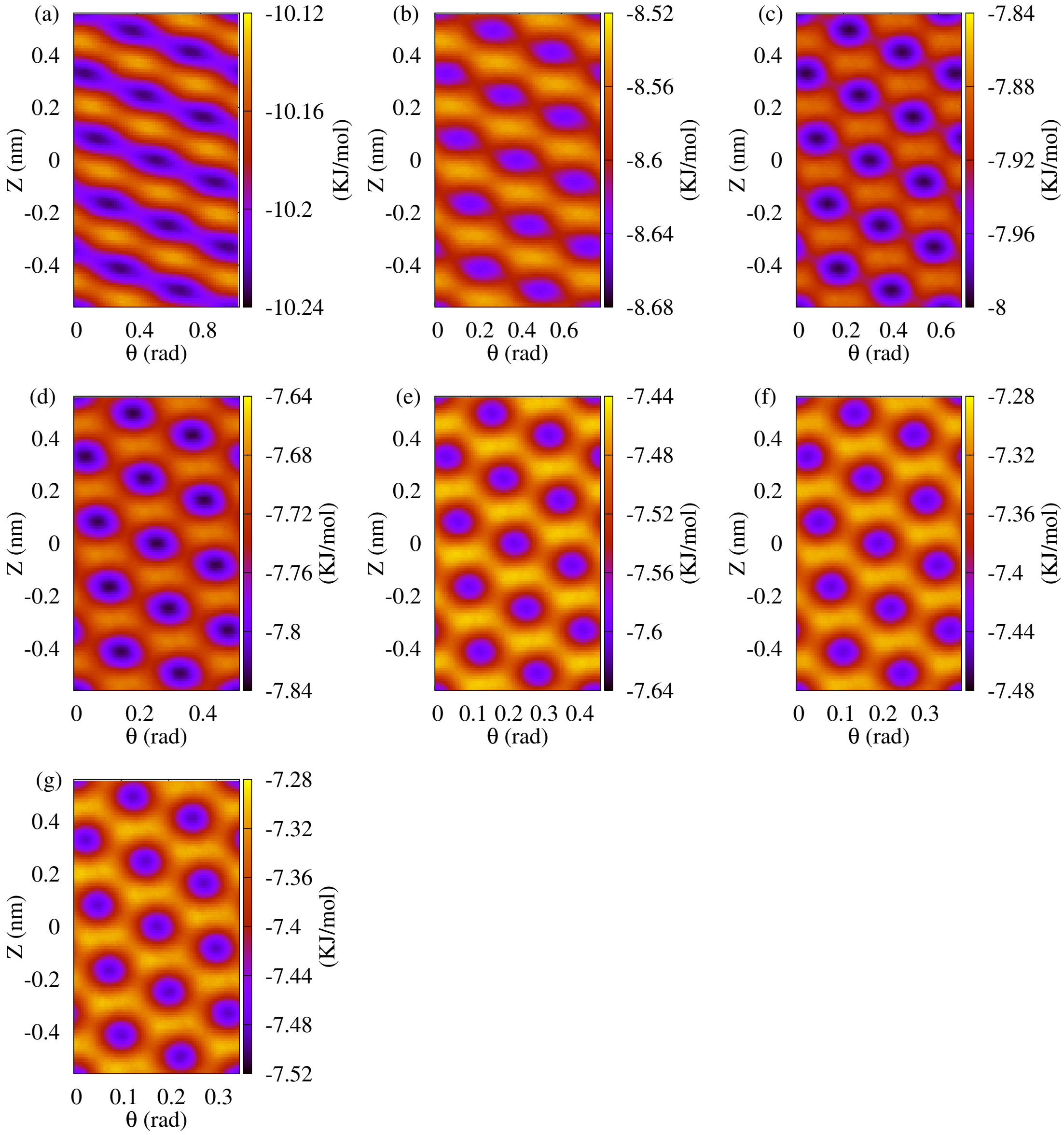

Fig. S 3 Potential energy landscapes between water and CNT with type (a) (6,12) at R=0.29 nm, (b) (8,16) at R=0.50 nm, (c) (10,20) at R=0.71 nm, (d) (12,24) at R=0.93 nm, (e) (14,28) at R=1.14 nm, (f) (16,32) at R=1.35 nm, and (g) (18,36) at R=1.57 nm.

4 FITTED POTENTIAL ENERGY LANDSCAPES BETWEEN CNT AND WATER MOLECULE

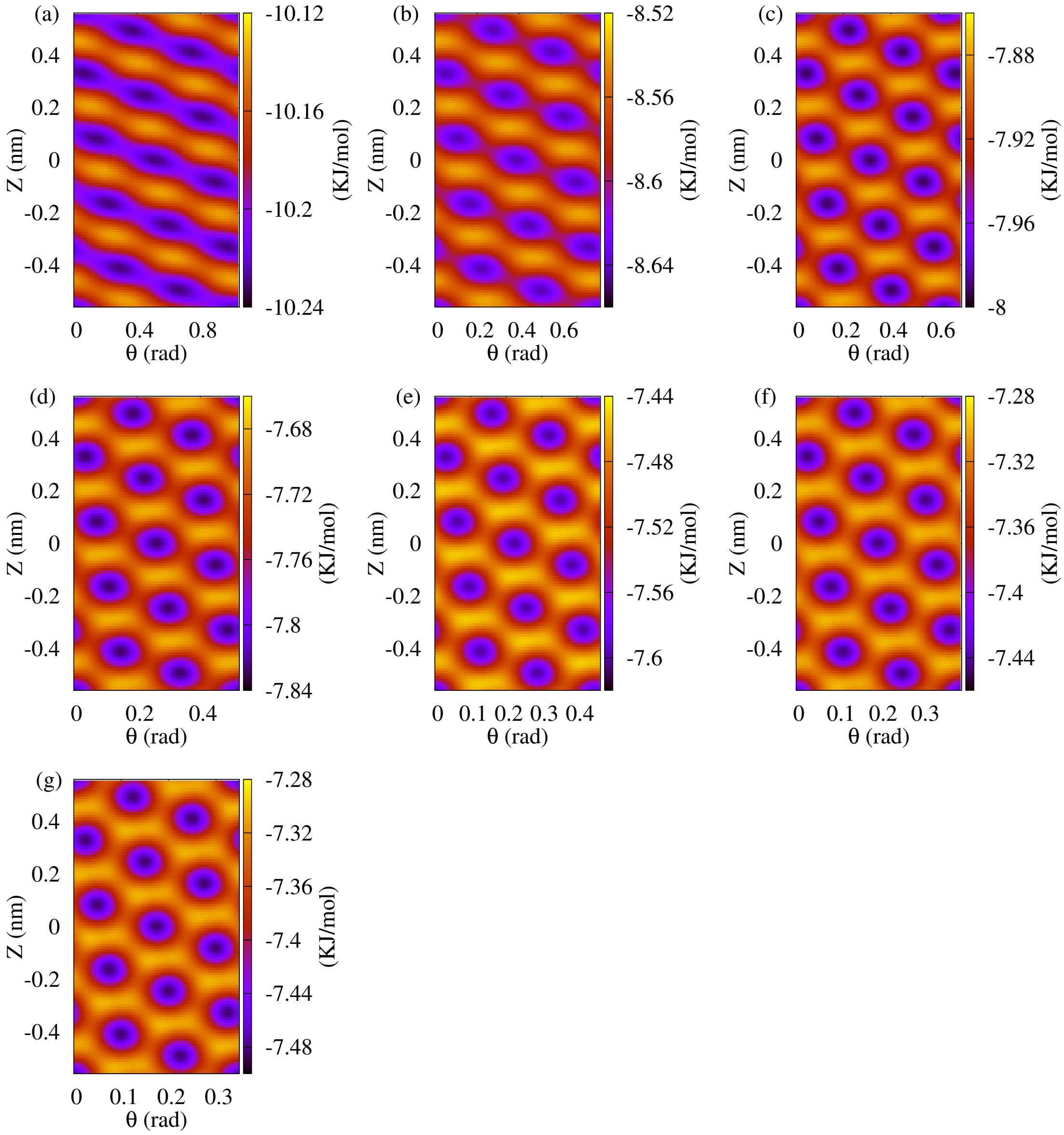

Fig. S 4 Fitted potential energy landscapes between water and CNT with type (a) (6,12) at R=0.29 nm, (b) (8,16) at R=0.50 nm, (c) (10,20) at R=0.71 nm, (d) (12,24) at R=0.93 nm, (e) (14,28) at R=1.14 nm, (f) (16,32) at R=1.35 nm, and (g) (18,36) at R=1.57 nm.

5 MEASUREMENT OF THE FRICTION COEFFICIENT OF THE CNT

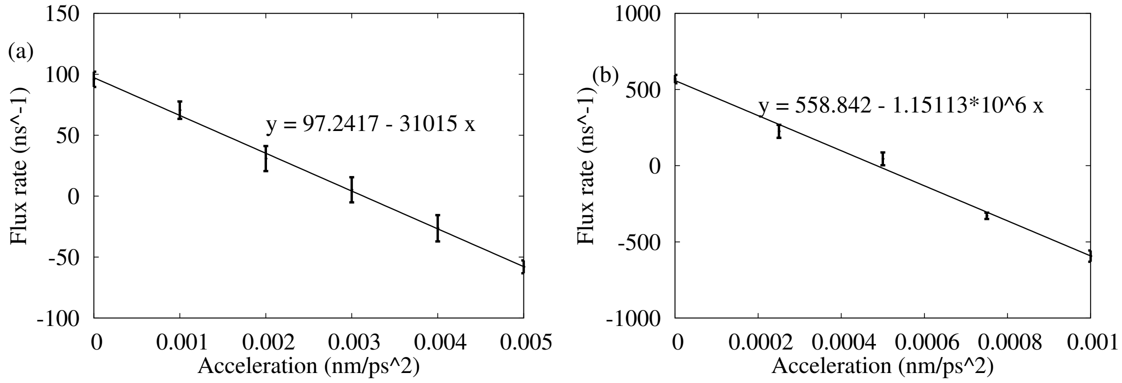

Fig. S 5 (a) Flux rate inside (6,12) CNT as a function of the acceleration. (b) Flux rate inside (14,28) CNT as a function of the acceleration.

6 ANGULAR VELOCITY OF WATER INSIDE (6,12) CNT

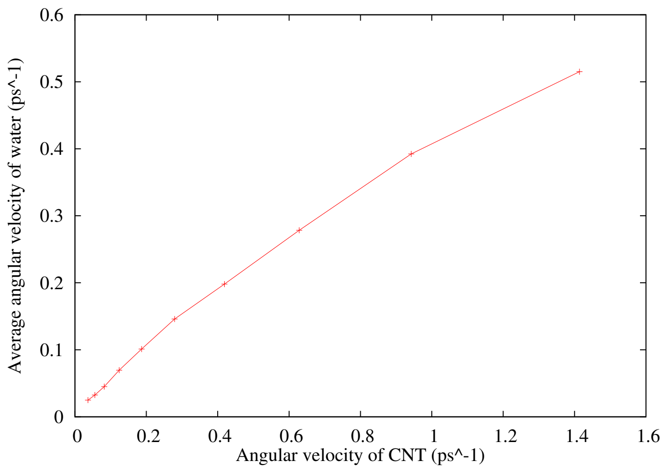

Fig. S 6 Angular velocity of water as a function of angular velocity of CNT.

7 ROBUSTNESS OF WATER FLUX AS A FUNCTION OF ANGULAR VELOCITY

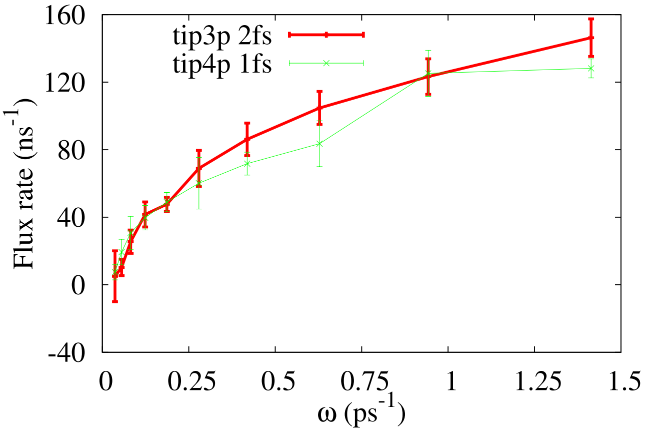

Fig. S 7 A comparison of water flux under TIP3P water model with timestep 2 fs and TIP4P water model with timestep 1 fs.

8 WATER FLUX AS A FUNCTION OF ANGULAR VELOCITY INSIDE (14,28) CNT

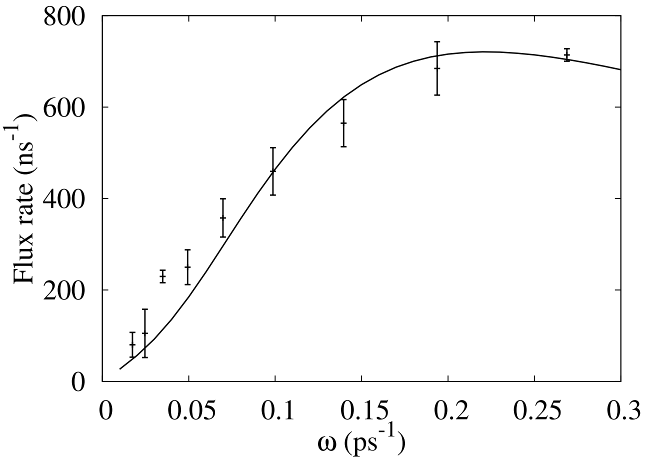

Fig. S 8 Flux rate inside a (14,28) CNT as a function of the angular velocity. Simulation results are dotted with errorbars and the line are fitted from the dragging theory.

9 AXIAL VELOCITY OF WATER

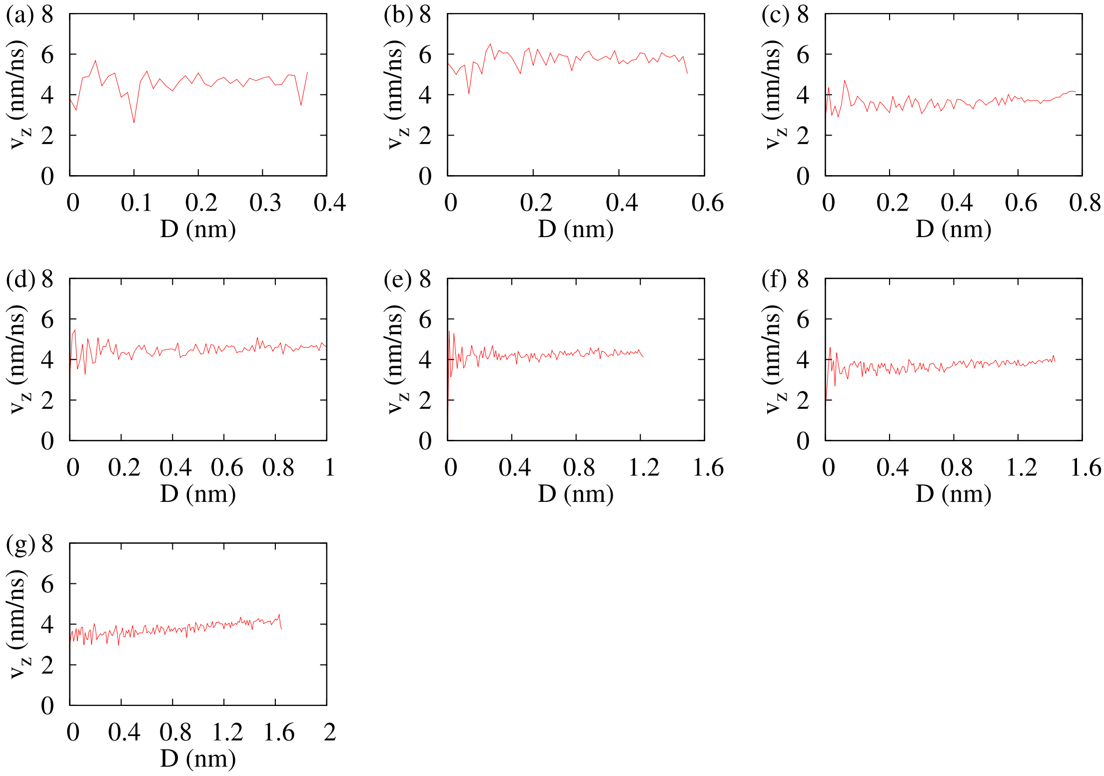

Fig. S 9 Axial velocity of water as a function of distance from the axis of the CNT with indices (a) (6,12), (b) (8,16), (c) (10,20), (d) (12,24), (e) (14,28), (f) (16,32), (g) (18,36).

10 METHODS FOR MODIFYING THE CNT

10.1 METHOD FOR MODIFYING THE CNT WITH CHARGE

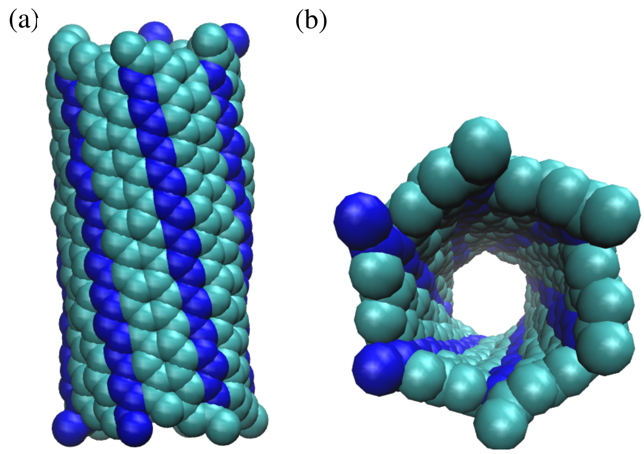

Fig. S 10 (a) Side and (b) top views of the electro-modified CNT. The carbon atoms carrying partial charge are colored in blue, and the neutral atoms in cyan.

10.2 METHOD FOR FUNCTIONALLIZING THE CNT

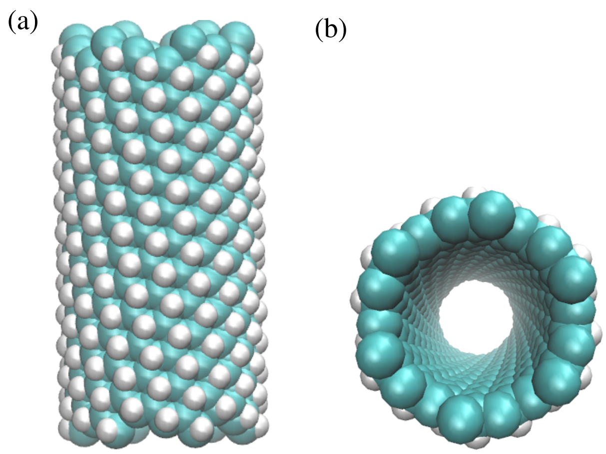

Fig. S 11 (a) Side and (b) top views of the functionalized CNT. The carbon atoms are colored in cyan, and the hydrogen atoms in white.