Supporting Material to

Selective Transport through the Ultra-Short Carbon Nanotubes Embedded in Lipid Bilayers

by

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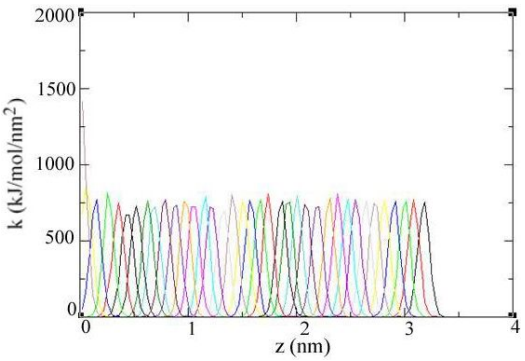

Figure S1. Umbrella histograms. The overlap between adjacent windows from approximate 0-3.4 nm of COM spacing is reasonable, and the umbrella sampling is sufficient.

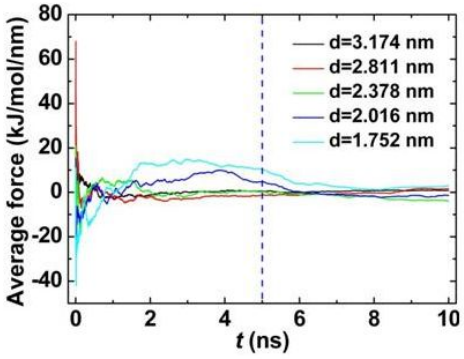

Figure S2. Cumulative average forces as a function of simulation time at five selected windows. As shown, the force curves in the last 5 ns are kept flat, indicating that umbrella sampling during the last 5 ns is well converged.

To investigate the effects of the conducting property of CNTs on the selective transport of polar molecules, we have constructed zigzag (10, 0), (12, 0) and (14, 0)

CNTs and rerun the systems B3, C3 and D3. The diameters of these CNTs fall in the range of 0.78~1.09 nm, in line with those of (6, 6), (7, 7) and (8, 8) CNTs.

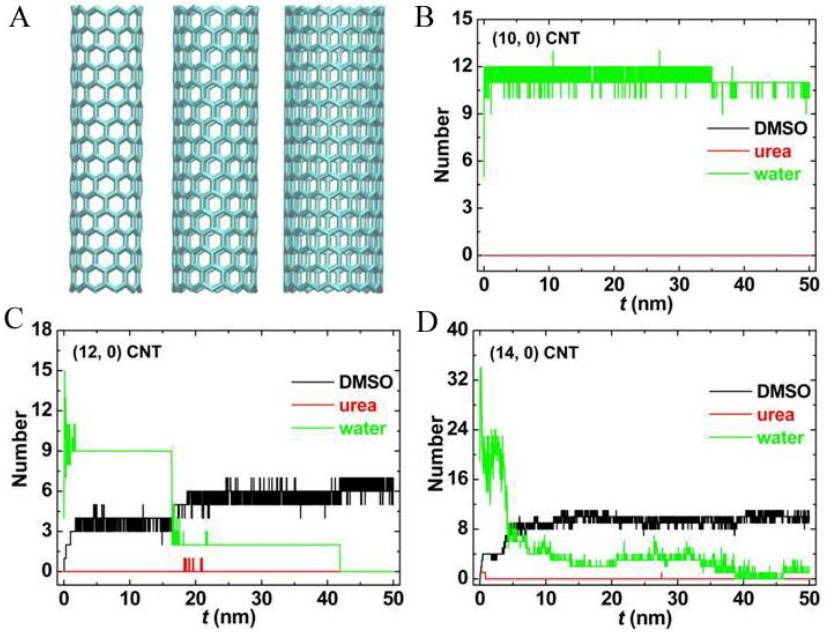

Figure S3. (A) Atomic structures of (10, 0), (12, 0) and (14, 0) CNTs. Their diameters fall in the range of 0.80~1.09 nm, close to those of (6, 6), (7, 7) and (8, 8) CNTs. (B-D) Number of DMSO, urea and water molecules within the three zigzag CNTs as a function of simulation time.

The transport of DMSO, urea and water molecules in the three zigzag CNTs presents the similar results with that in the armchair CNTs. As shown in Figure S3, DMSO and urea molecules cannot enter the (10, 0) CNT. With the increasing size, DMSO has priority to flow in the tube and accompanied by water molecules.

To investigate the effects of concentration on the selective transport of polar molecules through CNT hollow channels, we have rerun the systems B3, C3 and D3 at 5 mol% and 8 mol%. The results are presented in Figure S4.

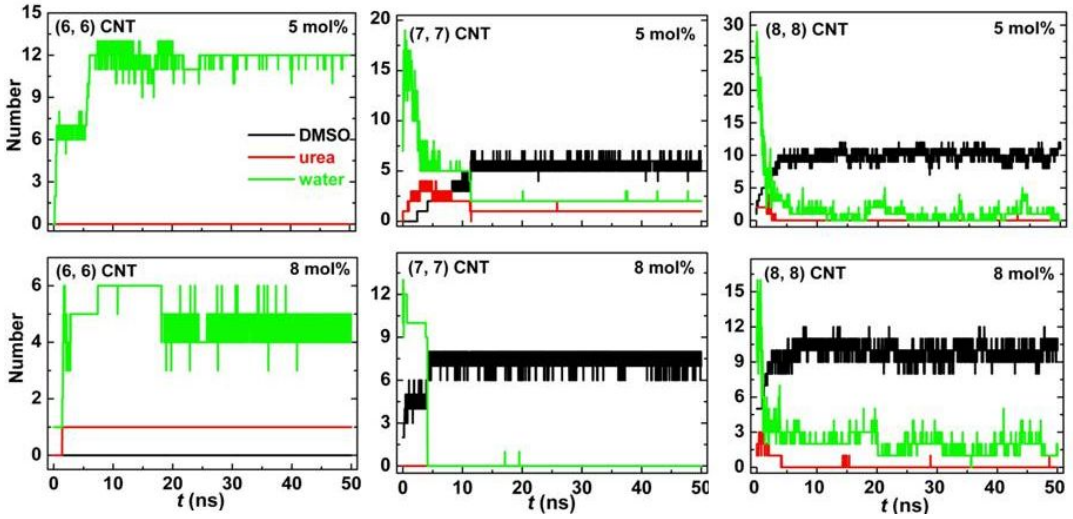

Figure S4. The number of DMSO, urea and water molecules in the (6, 6), (7, 7) and

(8, 8) CNTs at concentrations 5 mol% (*Upper*) and 8 mol% (*Lower*).

As we can see from Figure S4, DMSO and urea cannot enter the (6, 6) CNT. With the increasing size, DMSO has priority to flow in the tube and accompanied by water molecules, independent of their concentrations.

To investigate the effects of temperature on the selective transport of polar molecules through CNT hollow channels, we rerun the systems B3, C3 and D3 at 343 K and 363 K. The results are given in Figure S5.

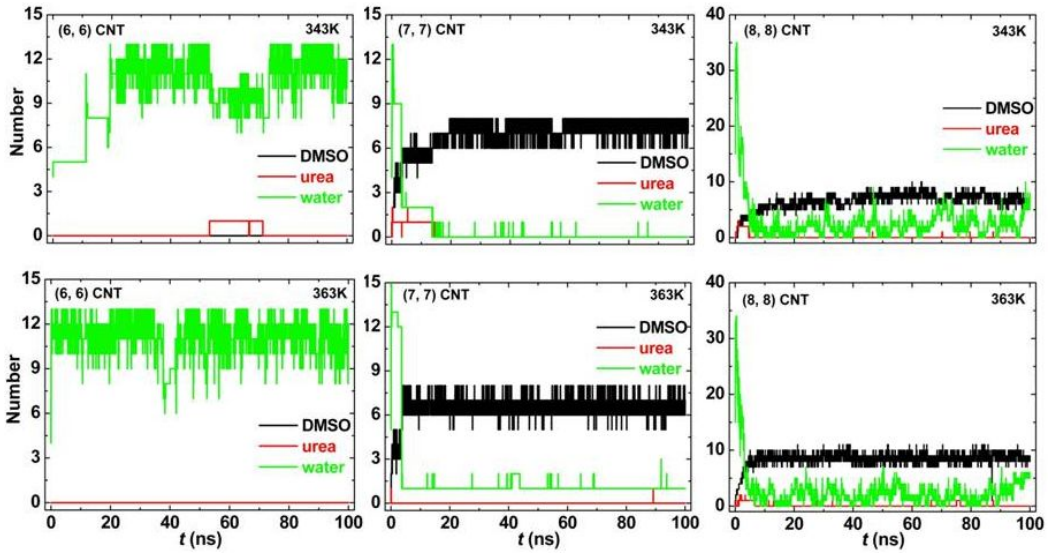

Figure S5. The number of DMSO, urea and water molecules in the (6, 6), (7, 7) and (8, 8) CNTs at 343 K (*Upper*) and 363 K (*Lower*).

DMSO and urea cannot enter the (6, 6) CNT. With the increasing size, DMSO has priority to flow in the tube and accompanied by water molecules, independent of the temperature.

We have also constructed three functionalized CNTs, terminated by hydroxyl groups, as shown in Figure S6. And then we rerun the systems B3, C3 and D3 with the three functionalized CNTs. The results are given in Figure S7.

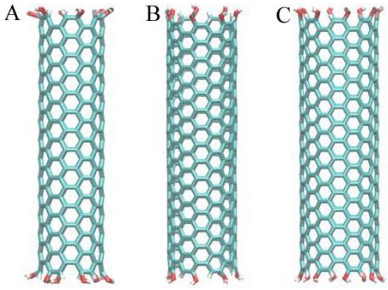

Figure S6. Atomic structure of (A) (6, 6) CNT-OH, (B) (7, 7) CNT-OH and (C) (8, 8) CNT-OH. Both ends are grafted with alternating hydroxyl and hydrogen termini.

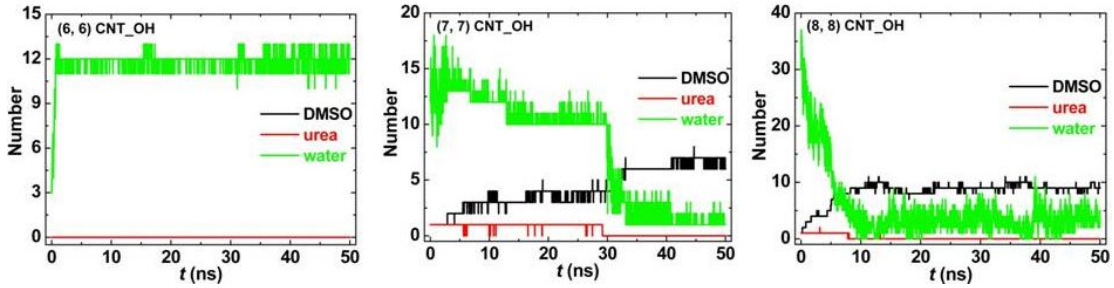

Figure S7. The number of DMSO, urea and water molecules in the functionalized (6, 6), (7, 7) and (8, 8) CNTs.

Similarly, DMSO and urea cannot enter the functionalized (6, 6) CNT. With the increasing size, DMSO has priority to flow in the tube and accompanied by water molecules. The functionalization has no effect on the selectivity of CNTs between DMSO and urea.

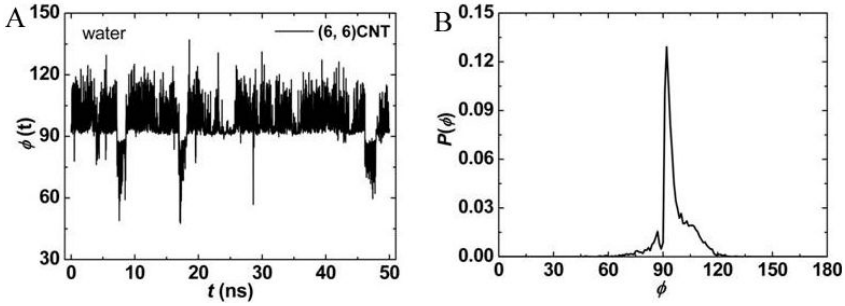

Figure S8. (A) Average dipole angle $\varphi(t)$ water molecules in the (6, 6) CNT. (B) The probability distribution $P(\varphi)$ of the average dipole angle $\varphi(t)$.

Figure S8 shows the results of the dipole angle and probability distribution of water molecules in (6, 6) CNT.