

Electronic Supplementary Information for

Tuning water transport through nanochannels by changing the direction of external electric field

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PS1: The dependences of $\langle \text{flux} \rangle$ on the strength of external electric field.

We show here the dependenc of $\langle \text{flux} \rangle$ on the strength of external electric field (figure S1 (a and b)). Comparing figure S1 (a) with figure 2, the similar changing trends of $\langle \text{flux} \rangle$ with the angle θ are observed under different strengths of external field (E).

From figure S1 (a) and figure 2, we can see that the $\langle \text{flux} \rangle$ under $E=0.5$ V/nm is smaller than that under $E=1$ V/nm. It is shown in figure S1 (b) that $\langle \text{flux} \rangle$ is monotonically increased with the strength of the external field. The inset of figure S1 (b) shows that as E decreases, the probability of bipolar orientation for the water molecules in CNT increases. The bipolar orientation may disrupt the unidirectional transport of the water molecules through the CNT. Furthermore, when E decreases to 0.2 V/nm, the probability of $-$ dipole state increases largely. The $-$ dipole state of the water molecules in CNT would result in a large instantaneous $\text{flux}_{\text{down}}$ and a small instantaneous flux_{up} . As a result, $\langle \text{flux} \rangle$ is monotonically increased with the strength of the external field.

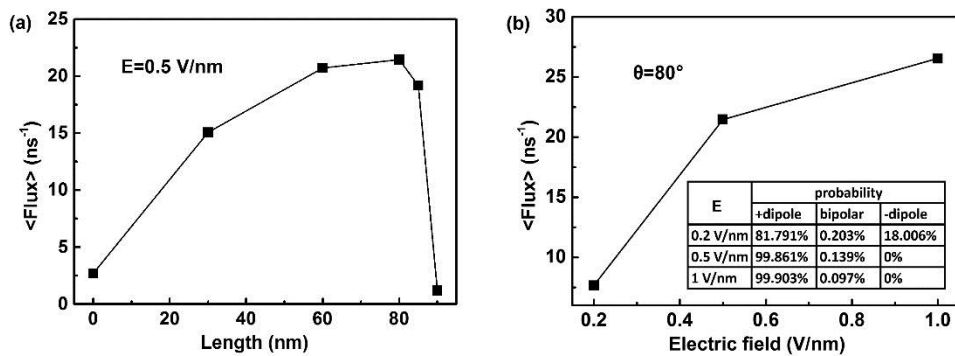


Figure S1. (a) The value of $\langle \text{flux} \rangle$ for different θ when the strength of the external field (E) is 0.5 V/nm . (b) The value of $\langle \text{flux} \rangle$ for different E when $\theta = 80^\circ$. Inset of (b): the probabilities for the +dipole state, the bipolar orientation, and the -dipole state, respectively. Each value of the $\langle \text{flux} \rangle$ was calculated from a 105 ns NVT molecular dynamics simulation. The last 100 ns trajectories were sampled for our analysis.