Electronic Supplementary Information

Accelerating water transport through a charged SWCNT: a molecular dynamics simulation

Diannan Lu*

Department of Chemical Engineering, Tsinghua University, Beijing, 10084

* Corresponding author: ludiannan@tsinghua.edu.cn

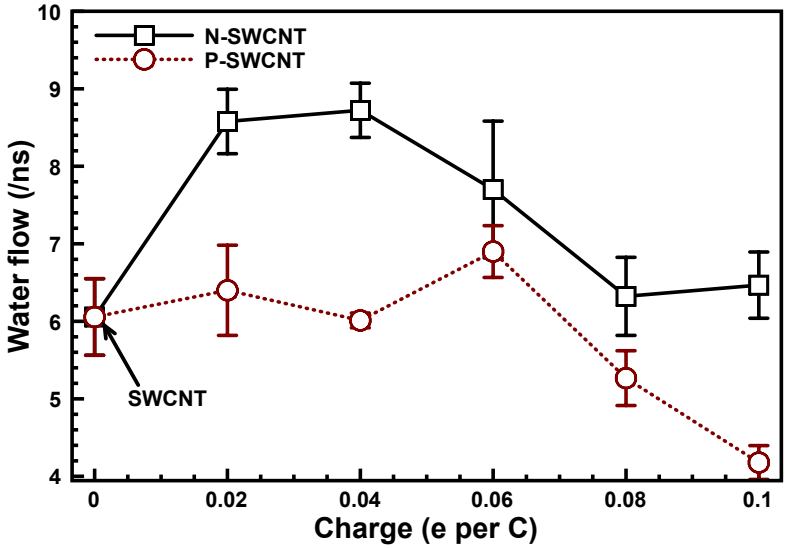

Figure S1. The water flow as a function of SWCNT surface charge

Water model is TIP3P.

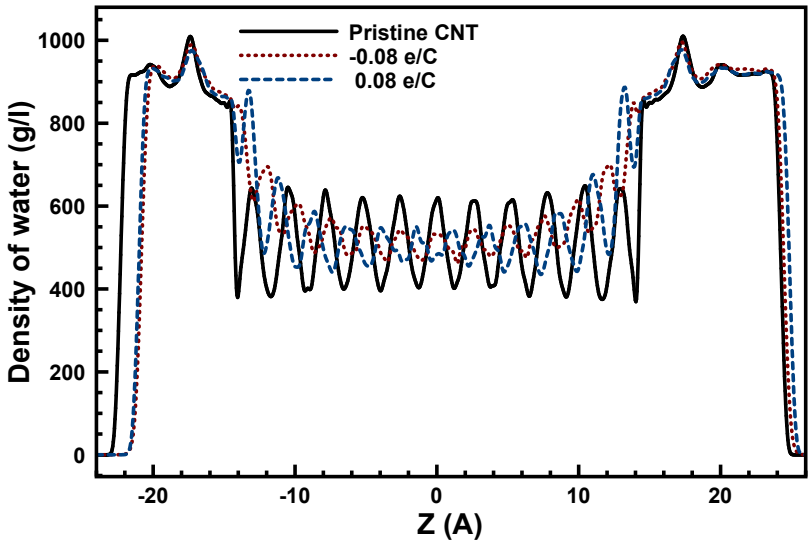

Figure S2. The density profile of water molecules inside carbon nanotubes of 3.0nm in length

Table S1. Water flow through different SWCNTs with 3.0nm in length

Charge (e/C)	Water flow (/ns)	Charge (e/C)	Water flow (/ns)
0.000 (Pristine)	1.408±0.266	0.000 (Pristine)	1.408±0.266
-0.025	1.558±0.072	0.025	1.392±0.201
-0.050	2.311±0.158	0.050	1.605±0.155
-0.080	2.397±0.562	0.080	1.311±0.517
-0.100	2.950±0.407	0.100	1.211±0.418

Table S2. Water flow through different SWCNTs with 5.0nm in length

Charge (e/C)	Water flow (/ns)	Charge (e/C)	Water flow (/ns)
0.000 (Pristine)	1.417±0.210	0.000 (Pristine)	1.417±0.210
-0.025	1.433±0.459	0.025	1.300±0.497
-0.050	1.883±0.429	0.050	1.350±0.082
-0.080	1.667±0.624	0.080	1.032±0.380
-0.100	0.950±0.236	0.100	0.536±0.209

Table S3 Water flow through different SWCNTs with different diameter

Format	Charge	Diameter (nm)	Area (nm^2)	Water flux (/ns)	Water flow (/ns□□□^{2})
(6, 6)	0.00	0.824	0.533	3.0	5.63
(6, 6)	-0.08	0.824	0.533	6.0	11.17
(11, 11)	0.00	1.510	1.791	151.2	84.42
(11, 11)	-0.08	1.510	1.791	220.3	123.00
(16, 16)	0.00	2.197	3.789	338.5	89.34
(16, 16)	-0.08	2.197	3.789	428.7	113.15
(21, 21)	0.00	2.884	6.528	539.8	82.70
(21, 21)	-0.00	2.884	6.528	552.0	84.56