Supplementary Information for "Water transport through nanotubes with varying interaction strength between tube wall and water" by Mathhew Melillo, Fangqiang Zhu, Mark A. Snyder, and Jeetain Mittal*

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1. *Lennard-Jones Potential between nanotube atoms and water*

The Lennard-Jones Potential is a model to describe the interactions between a nanotube atom (NT) and water's oxygen atom (OW). The interaction energy depends on the distance between the two atoms in question, r, as well as the parameters of ε_{NT-OW} and σ_{NT-OW}. Here, ε_{NT-OW} represents the potential energy well depth, which is the point at which the molecules or atoms are a distance of r_{min} from each other and have potential energy, $U=-\varepsilon_{NT-OW}$. The resulting potential functions are also shown in Figure S1.

Table1. Lennard-Jones potential parameters used

ε_{NT-OW} (kcal/mol)	r_{min} (Å)	σ_{NT-OW} (Å)
0.0200	4.1812	3.7250
0.0400	3.9679	3.5350
0.0500	3.9000	3.4745
0.0525	3.8875	3.4634
0.0550	3.8750	3.4522
0.0575	3.8625	3.4411
0.0600	3.8500	3.4300
0.0625	3.8350	3.4166
0.0650	3.8250	3.4077
0.0675	3.8200	3.4032
0.0700	3.8100	3.3943
0.0725	3.8000	3.3854
0.0750	3.7900	3.3765
0.0775	3.7800	3.3676
0.0800	3.7715	3.3600
0.1000	3.7154	3.3100
0.1200	3.6648	3.2650
0.1400	3.6256	3.2300
0.1600	3.5919	3.2000
0.1800	3.5638	3.1750
0.2000	3.5414	3.1550

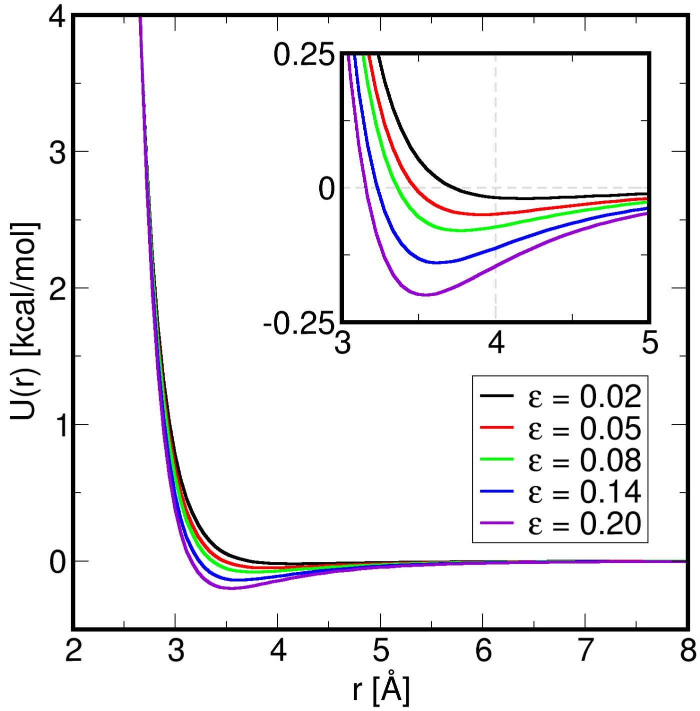

Figure S1: Potential energy U(r) versus distance between a nanotube atom and water's oxygen for different $\varepsilon_{NT\text{-}OW}$ values (the inset shows a zoomed-in view).

2. *Comparison of permeation events between our membrane system (3x4 nanotubes) and a single nanotube system*

To verify that the membrane system used to accumulate data doesn't affect our results for flow through a nanotube, we have also performed a set of simulations with a setup utilizing a single nanotube (6,6) immersed in water. As we show in Figure S2, the results are comparable between the 'membrane' and 'single tube' simulation setups.

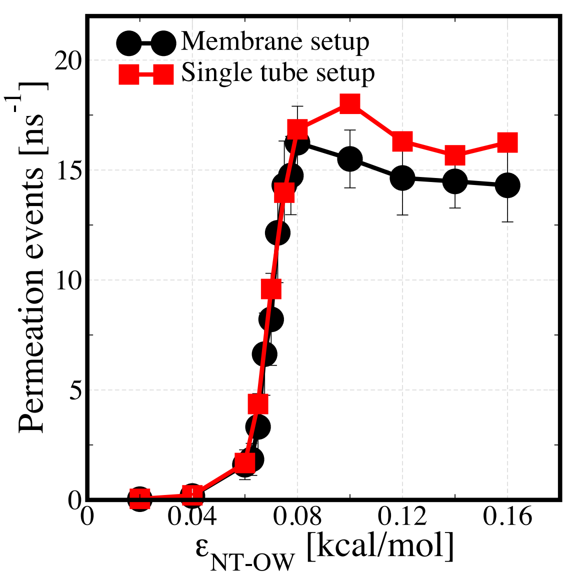

Figure S2: Effect of system setup, membrane versus single nanotube, on observed water flow through a nanotube.

3. *Effect of changing* $\sigma_{NT\text{-}OW}$ *for a given interaction strength* $\varepsilon_{NT\text{-}OW}$

Consistent with previous studies [1-3], we have changed the nanotube atom's diameter for different $\varepsilon_{NT\text{-}OW}$ to make sure that repulsive part of the potential (Figure S1) is the same. To see how keeping this diameter or therefore $\sigma_{NT\text{-}OW}$ constant ($\sigma_{NT\text{-}OW}$ = 3.2751 Å which corresponds to carbon nanotube as used previously in the literature) for different $\varepsilon_{NT\text{-}OW}$ values will (not) affect our results, we have generated a data set for (6,6) nanotubes. As shown below in Figure S3, the permeation events are largely insensitive to this change.

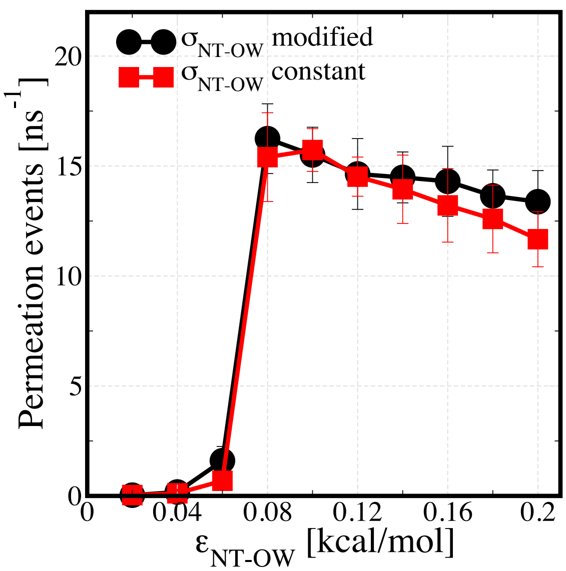

Figure S3: Effect of $\sigma_{NT\text{-}OW}$ (see section 1) on observed permeation rates.

4. *Simulation setup details*

Table2. List of simulation systems and runtime considered in this study

Nanotube (n,m)	Length (nm)	$\varepsilon_{NT\text{-}OW}$ range (kcal/mol)	Equilibration time (ps)	Production time (ns)	Number of water molecules
(6,6)	1.34	0.02-0.2	200	15	1541
(7,7)	1.34	0.02-0.2	200	15	1924
(8,8)	1.34	0.02-0.2	200	15	2346
(9,9)	1.34	0.02-0.2	200	15	2910
(12,12)	1.34	0.02-0.2	200	15	4972
(12,12)	1.34	0.04-0.06	200	100	4972
(6,6)	5.6	0.02-0.2	400	30	1706