Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

for

Resistance of Water Transport in Carbon Nanotube Membranes

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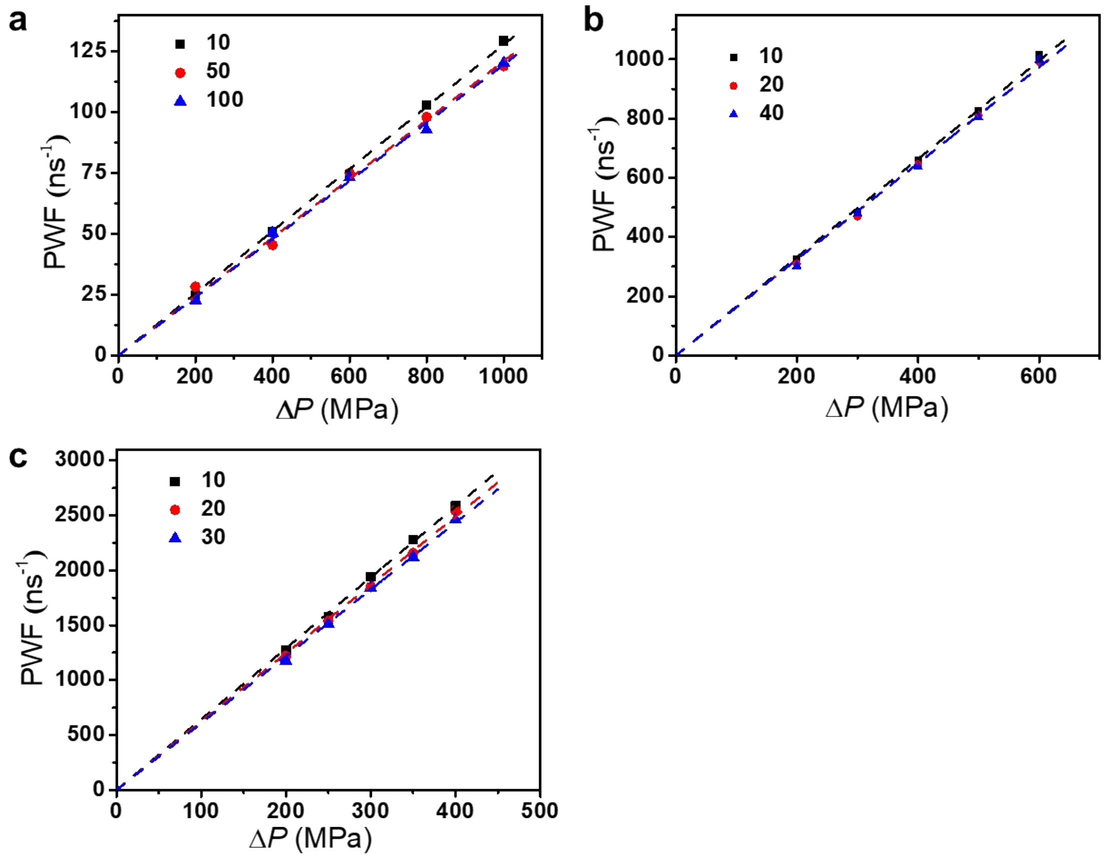

Figure S1. PWF at different Δ*P*s of normal water transport through CNT membranes: (a) (6,6) CNTs with the length of 10, 50, and 100 nm; (b) (10,10) CNTs with the length of 10, 20, and 40 nm; (c) (14,14) CNTs with length of 10, 20, and 30 nm.

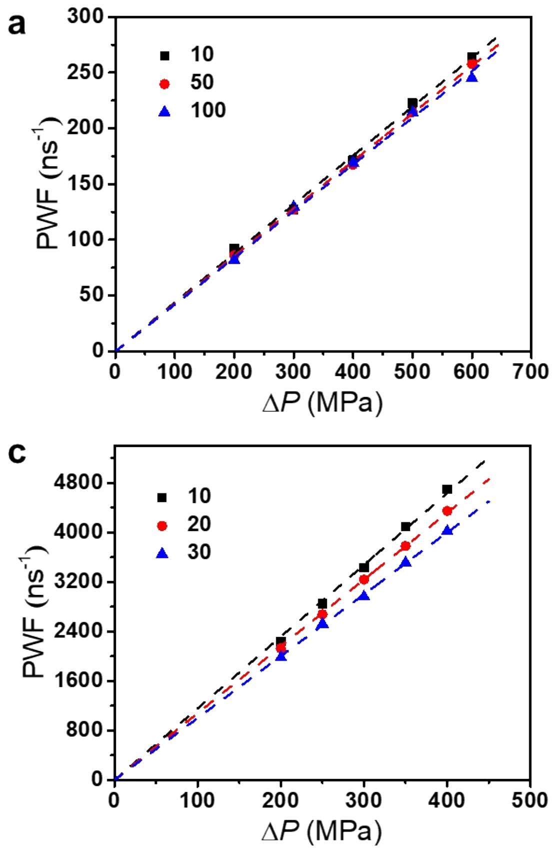

Figure S2. PWF at different ΔPs of apolar water transport through CNT membranes: (a) (6,6) CNTs with the length of 10, 50, and 100 nm; (b) (10,10) CNTs with the length of 10, 20, and 40 nm; (c) (14,14) CNTs with length of 10, 20, and 30 nm.

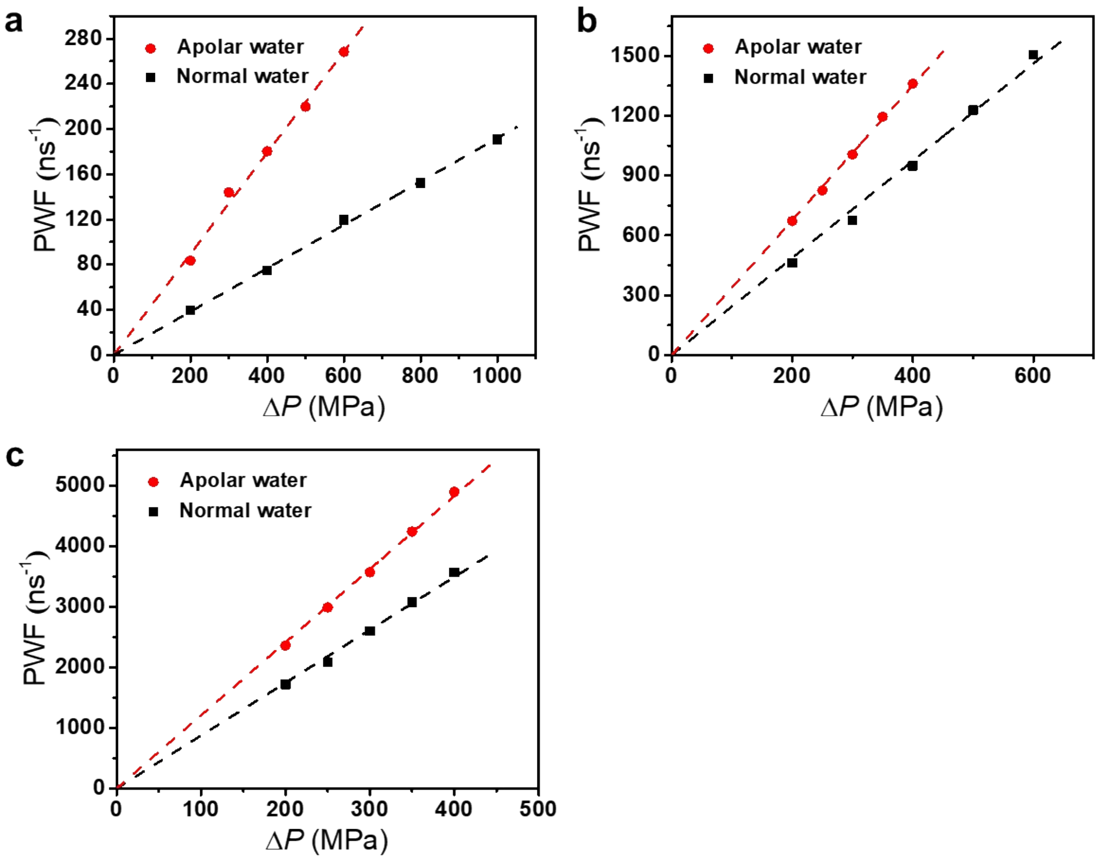

Figure S3. PWF at different Δ*P*s of apolar and normal water in (6,6) (a), (10,10) (b), and (14,14) (c) CNT membranes with hourglass-shaped pore mouth.

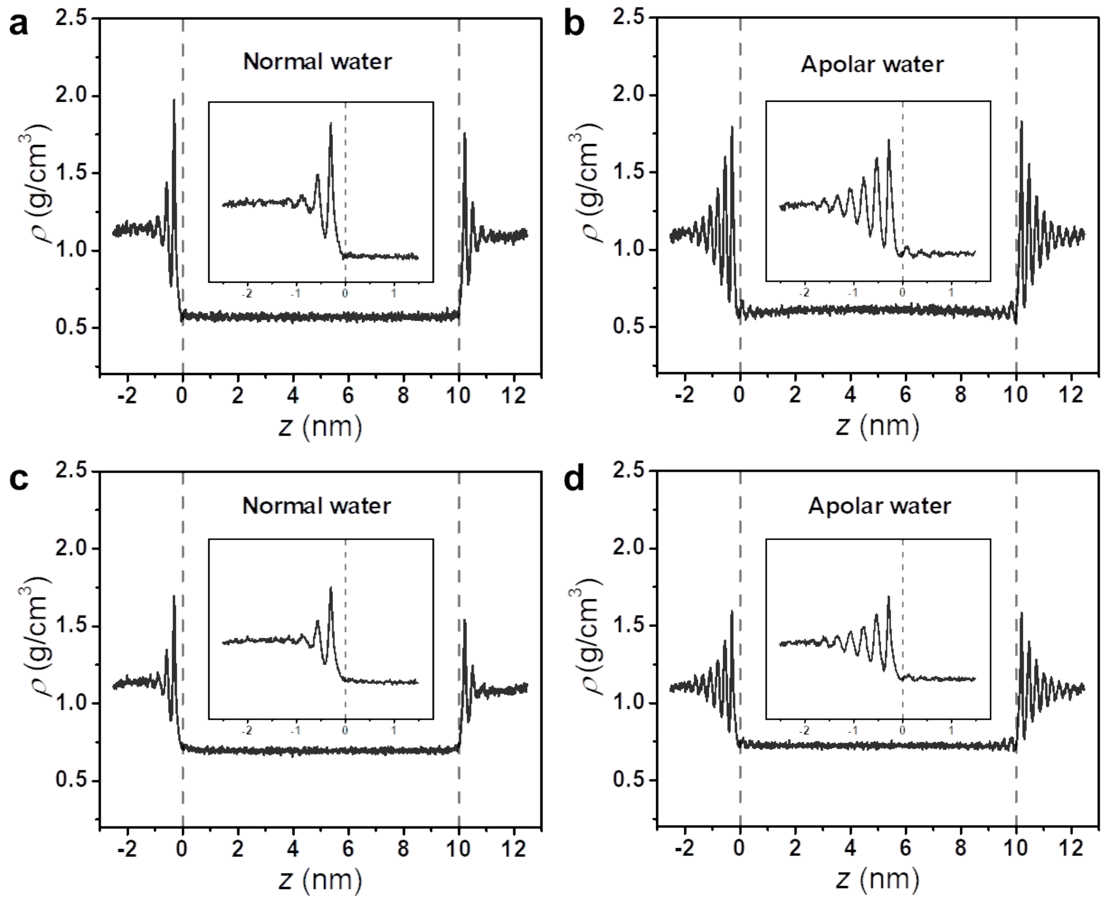

Figure S4. Density profiles in the selected region along *z* axis of (10,10) (water a and b) and (14,14) (water c and d) CNT membranes. The region of CNT and its elongate region into water reservoirs are selected, i.e. the region where the perpendicular graphene sheets located is excluded. Two gray dashed lines represent the entrance and exit of the membrane. The insets are amplificatory patterns of the entrance region.

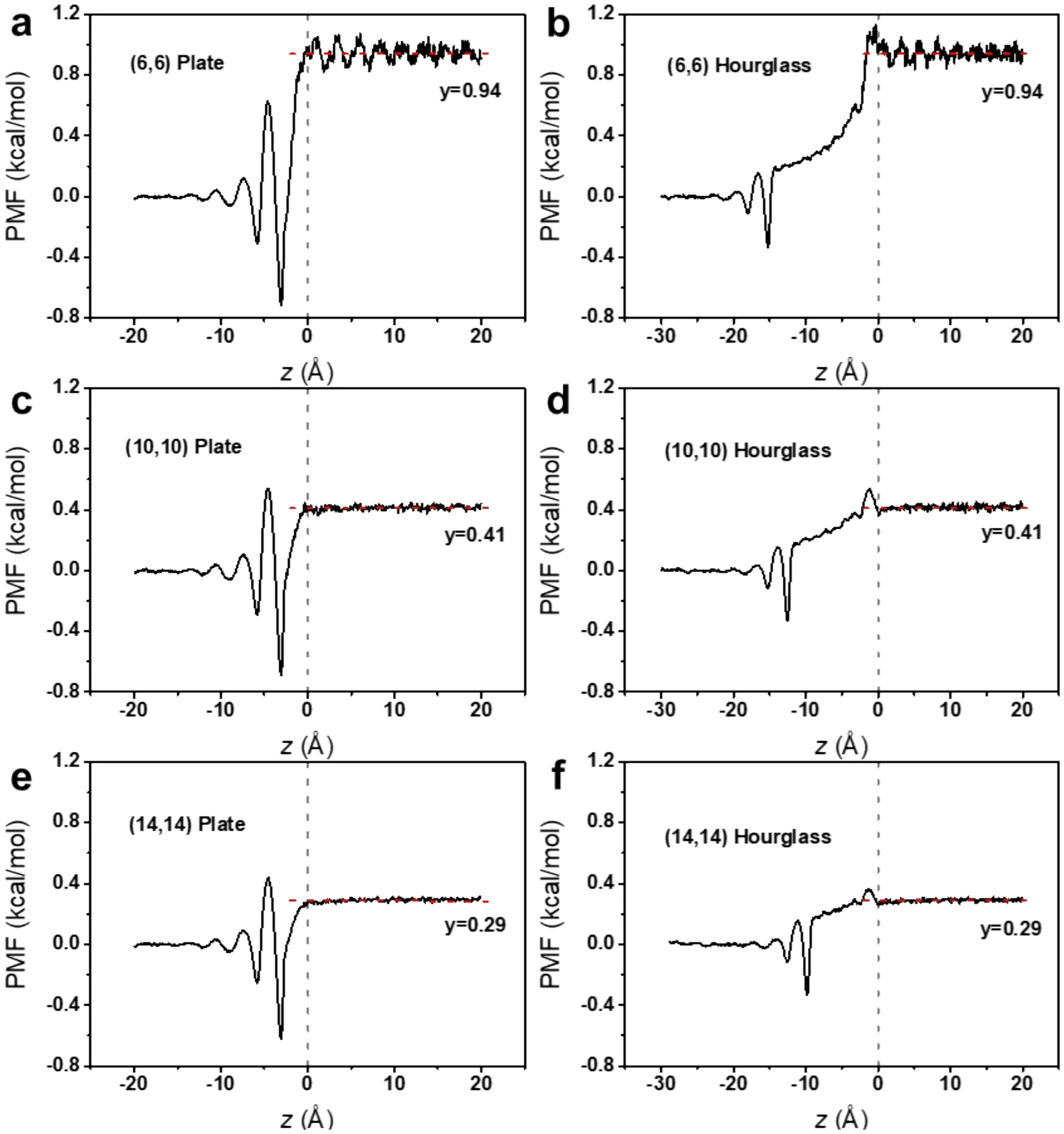

Figure S5. PMF profiles for water transport along *z* axis around the plate-shaped (a, c, and e) or hourglass-shaped (b, d, and f) entrance region of (6,6), (10,10), and (14,14) CNT membranes, respectively. The gray dashed line represents the entrance of the membrane.

The analysis of energy barriers around the entrance region

The potential of mean forces (PMFs) on water molecules passing through the entrance along z axis under equilibrium conditions were calculated by $\mathrm{PMF}(z) = -RT\ln(\rho(z)/\rho_0)$, where R is the gas constant, T is the temperature and $\rho(z)$, ρ_0 is the density of water at z position and in bulk, respectively.[1, 2] The calculated energy barrier is often used to evaluate the blocking capability of water channels. As shown in Fig. S5, the energy barrier decreases from 0.94 to 0.29 kcal/mol with increased diameters because of the less confined environment of CNTs. Then, compared to the plate-shaped pore mouth, CNT membranes with the hourglass-shaped pore mouth have nearly the same high energy barrier, which indicates that the blocking effect to water molecules is unchanged. But in our analysis of the water transport resistance, the $R_{\mathrm{interfacial}}$ is significantly reduced by the hourglass-shaped pore mouth. The reason may be that the energy barrier is not directly related to the transport resistance. The major difference between them may be that the energy barrier is a function of the state while transport resistance depends on the transport process. That is, the energy barrier just evaluates the blocking capability of water channels, but it cannot describe the transport process like the transport resistance.

Table S1. The total number of water molecules in each system.

CNT Dia. (nm)	l_{mem}[a] (nm)	No. waters (normal water)	No. waters (apolar water)
(6,6) 0.81	10	1932	1952
	50	2092	2192
	100	2292	2492
(10,10) 1.35	10	2162	2180
	20	2432	2468
	40	2972	3044
(14,14) 1.90	10	2544	2570
	20	3196	3248
	30	3848	3926

[a] l_{mem} is the membrane thickness in the unit of nm, which corresponds to the CNT length in this work.

Table S2. Resistance summary of CNT membranes.

CNT Dia. (nm)		R_{total} ($\times10^{11}$ m^{-1})			R_{interior} ($\times10^{9}$ m^{-1})	$R_{\text{interfacial}}$ ($\times10^{11}$ m^{-1})
(6, 6) 0.81	l_{mem}[a]	10	50	100	10	
	Normal[b]	31.2	33.0	33.4	25.2	31.2
	Apolar[b]	9.09	9.35	9.52	4.91	9.06
(10, 10) 1.35	l_{mem}	10	20	40	10	
	Normal	2.40	2.46	2.46	2.43	2.38
	Apolar	1.14	1.25	1.45	10.3	1.04
(14, 14) 1.90	l_{mem}	10	20	30	10	
	Normal	0.618	0.641	0.656	1.88	0.601
	Apolar	0.345	0.370	0.399	1.93	0.332

[a] l_{mem} is the membrane thickness in the unit of nm, which corresponds to the CNT length in this work.

[b] Normal and apolar represent the normal water and the apolar water, respectively.

References

1. B. Corry, *Journal of Physical Chemistry B*, 2008, **112**, 1427-1434.

2. Y. G. Yan, W. S. Wang, W. Li, K. P. Loh and J. Zhang, *Nanoscale*, 2017, **9**, 18951-18958.