Water Desalination using Graphene Nanopores: Effect of Water Models used in Simulations

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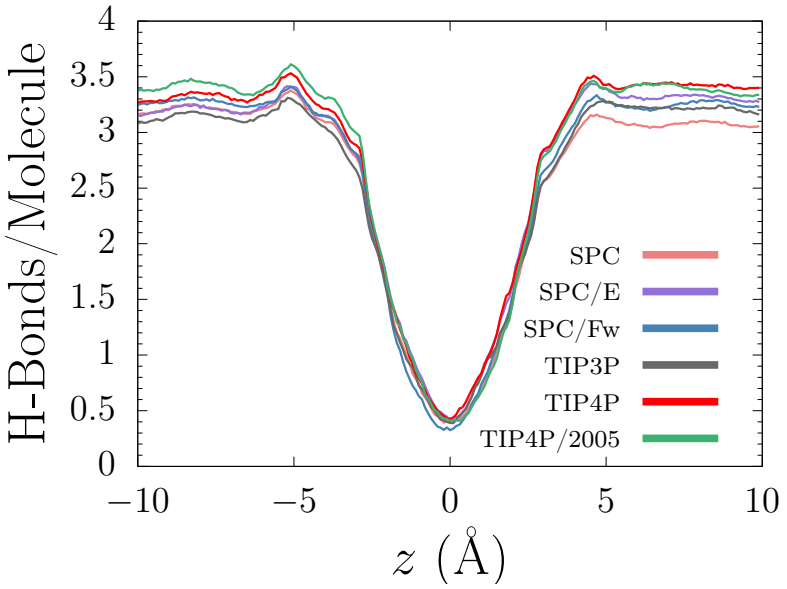

Figure S1: The number of hydrogen bonds per molecule along the pore axis. The pore is located at z=0.

Figure S1 shows the number of hydrogen bonds per molecule along the pore axis [1]. The number of hydrogen bonds per molecule reduces near the pore sheet while maintaining a constant value in the bulk. The hydrogen bonding between the water molecules is only considered in the analysis.

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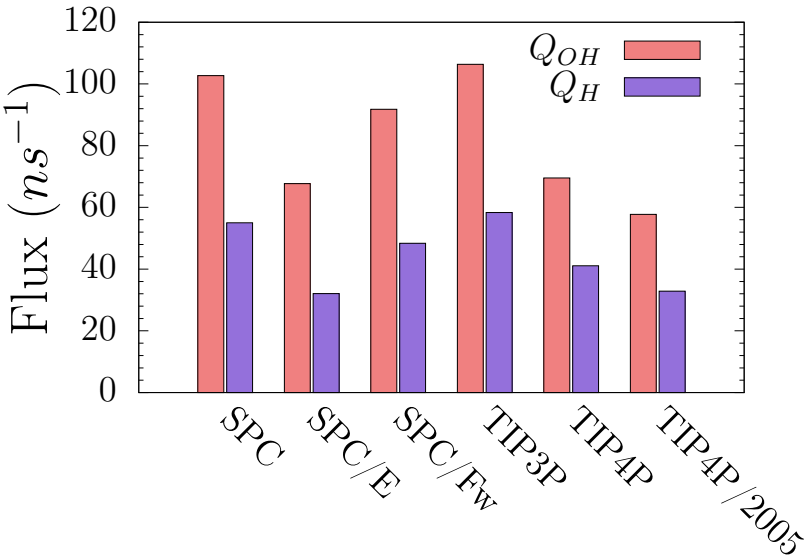

Figure S2: The variation in the flux between hydroxyl and hydrogen functionalized nanopores. The values are the average of three independent simulations.

Figure S2 shows the variation in flux between the hydroxyl (28 $Å^2$) and hydrogen (23 $Å^2$) functionalized nanopores. The results are in agreement with Tanugi and Grossman [2].

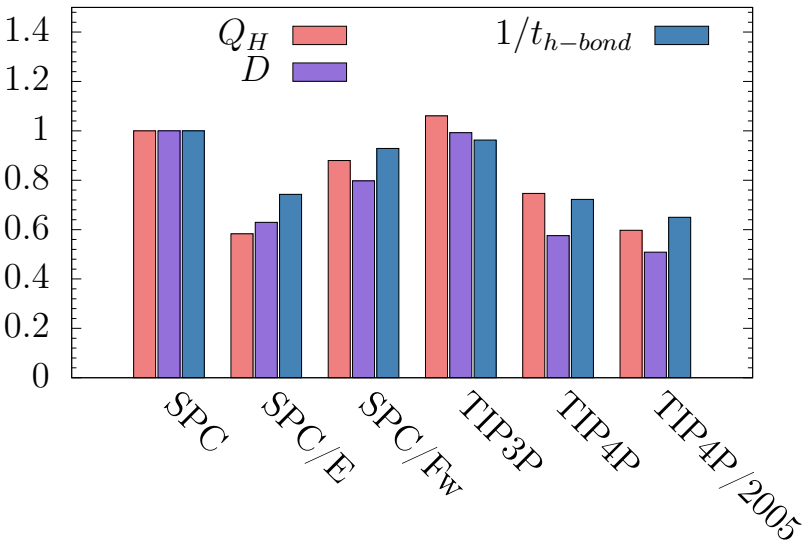

Figure S3: The correlation between the flux obtained using hydrogen functionalized pores, the diffusion coefficient and the hydrogen bond lifetime. The values are normalized with SPC. The hydrogen bond lifetime is inverted to illustrate the correlation better.

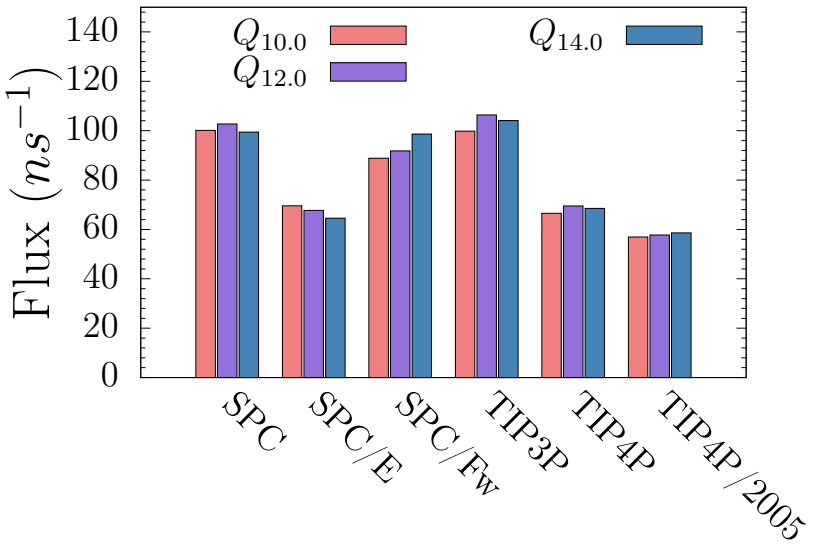

Figure S4: The variation of flux obtained using different cutoff values (10.0, 12.0 and 14.0 Å). The values are the average of three independent simulations.

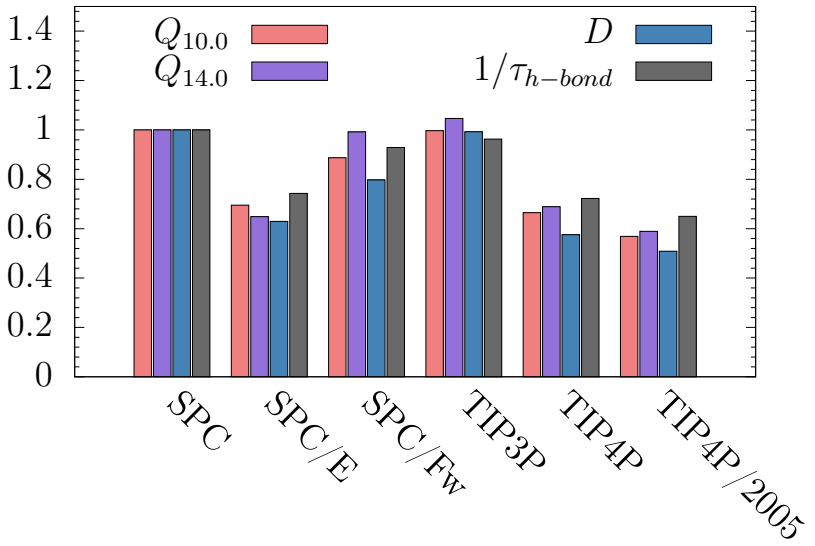

Figure S5: Correlation between the fluxes obtained using cutoffs 10.0 and 14.0 Å.

Table S1

Region	Water Model	A_1	τ_1	τ_2
Bulk	SPC	0.29 (0.01)	0.06 (0.00)	0.35 (0.00)
	SPC/E	0.27 (0.01)	0.08 (0.00)	0.46 (0.00)
	SPC/Fw	0.26 (0.01)	0.06 (0.00)	0.37 (0.00)
	TIP3P	0.28 (0.01)	0.06 (0.00)	0.35 (0.00)
	TIP4P	0.25 (0.02)	0.07 (0.00)	0.45 (0.01)
	TIP4P/2005	0.26 (0.02)	0.08 (0.00)	0.51 (0.01)
Interface	SPC	0.34 (0.03)	0.06 (0.00)	0.35 (0.03)
	SPC/E	0.38 (0.03)	0.07 (0.00)	0.42 (0.02)
	SPC/Fw	0.37 (0.03)	0.06 (0.00)	0.33 (0.01)
	TIP3P	0.37 (0.03)	0.06 (0.00)	0.35 (0.02)
	TIP4P	0.45 (0.04)	0.10 (0.01)	0.47 (0.02)
	TIP4P/2005	0.44 (0.02)	0.09 (0.00)	0.48 (0.02)
Pore	SPC	18.63 (5.72)	0.13 (0.02)	0.42 (0.04)
	SPC/E	7.97 (3.63)	0.11 (0.01)	0.53 (0.05)
	SPC/Fw	10.07 (3.77)	0.07 (0.01)	0.36 (0.03)
	TIP3P	9.28 (3.80)	0.11 (0.01)	0.40 (0.03)
	TIP4P	14.17 (4.49)	0.12 (0.02)	0.65 (0.08)
	TIP4P/2005	6.65 (2.72)	0.10 (0.02)	0.75 (0.07)

Table S1 shows the fitting parameters obtained for equation 5 using different water models in three regions. The values in the parenthesis indicate the standard error.

References

[1] Andrew M. Prpich, Yuebiao Sheng, Wei Wang, M. Elias Biswas, and P. Chen. Tension at the surface: Which phase is more important, liquid or vapor? *PLoS ONE*, 4(12):e8281, dec 2009.

[2] David Cohen-Tanugi and Jeffrey C. Grossman. Water desalination across nanoporous graphene. *Nano Lett.*, 12(7):3602–3608, jul 2012.