Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Polyoxometalate ionic liquid between graphene oxide surfaces as a new membrane in desalination process: A molecular dynamics study

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Table S1. The Dreiding non-bonded parameters

	mass	charge	σ (Å)	ε (kcal/mol)
C_2, Carbon(SP^2)	12.011	0	3.55	0.07
C_3, Carbon(C bonded to OH)	12.011	0.15	3.55	0.07
OH (O in OH group)	15.9994	-0.585	3.07	0.1699
HO (H in OH group)	1.008	0.435	0	0

Table S2. Bond stretching parameters (harmonic potential)*

i	j	r_o (Å)	k_b (kcal/mol Å^2)
C_2	C_2	1.33	1400.0
C_3	C_3	1.53	700.0
C_3	OH	1.42	700.0
OH	HO	0.98	700.0

Table S3. Angle bending parameters (hcos potential)*

i	j	k	θ_o(deg)	k_θ (kcal/mol)
C_2	C_2	C_3	120	133.33
C_2	C_2	C_2	120	133.33
C_2	C_3	C_3	109.47	112.49
C_3	OH	HO	104.51	106.69
C_3	C_3	OH	109.47	112.49
C_2	C_3	OH	109.47	112.49

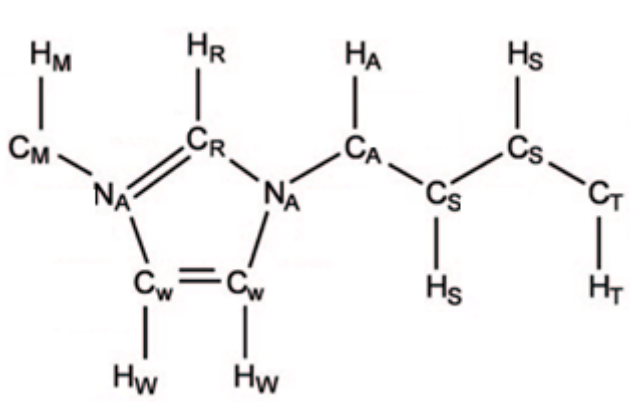
Table S4. Dihedral parameters (cos potential)*

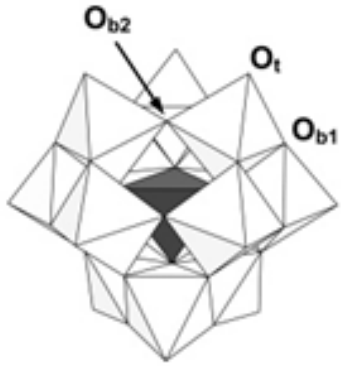
	l	A (kcal/mol)	m	δ
	C_2	1.25	180.0	2.0
	C_2	1.25	180.0	2.0
	C_2	0.11	0.0	3.0
	C_3	0.083	-180.0	6.0
	OH	0.11	0.0	3.0
	HO	0.33	0.0	3.0

* The dihedral parameters have been produced using the gui utility of DLPOLY software in which some parameters may be different according to the positions of atoms or kinds of bonds.

Table S5. The LJ parameters of the cation and anion of the polyoxometallate IL used in this work

	Charge (e)	ε (kcal/mol)	σ (Å)
P	1.51	0.2455	3
W	3.81	0.221292	2.34
Obt	-0.85	0.214713	3.17
Ob1	-1.37	0.214713	3.17
Ob2	-1.55	0.214713	3.17
CR	-0.11	0.07	3.55
NA	0.15	0.17	3.25
HW=HR	0.21	0.03	2.42
CM	-0.17	0.066	3.5
HM=HA=HT=HS	0.13	0.03	2.5
CW	-0.13	0.066	3.5





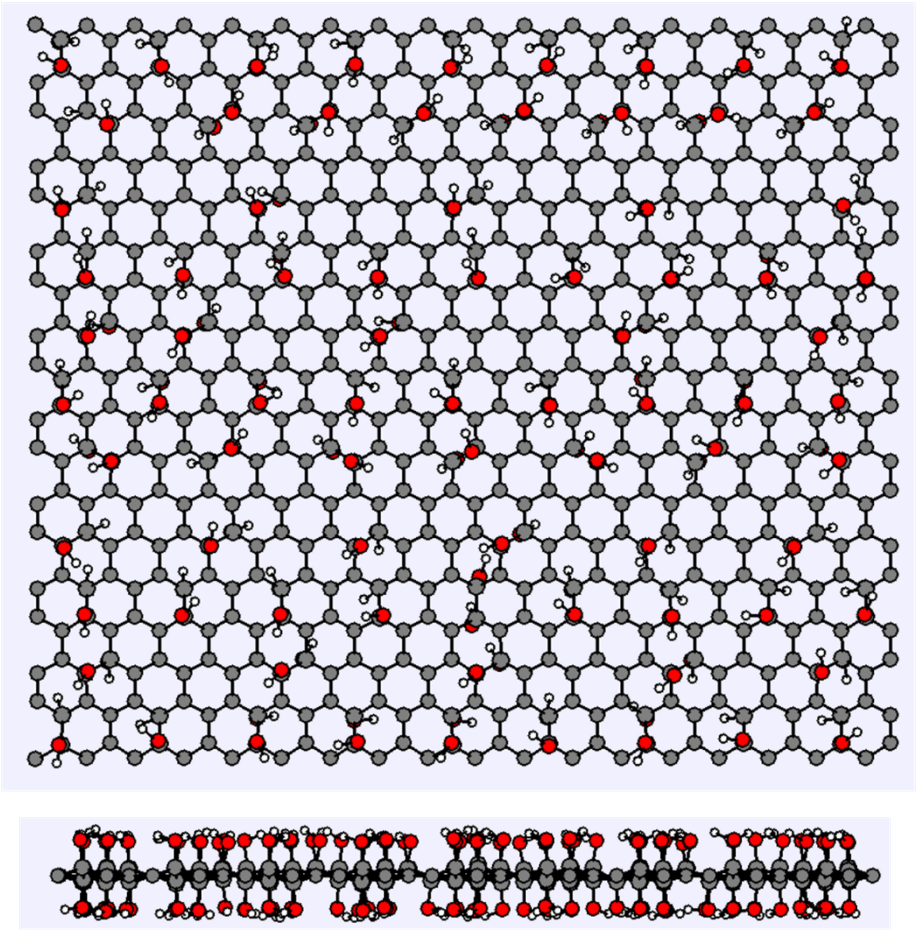


Fig. S1. The snapshots of the GO surface used in the simulations of this work.

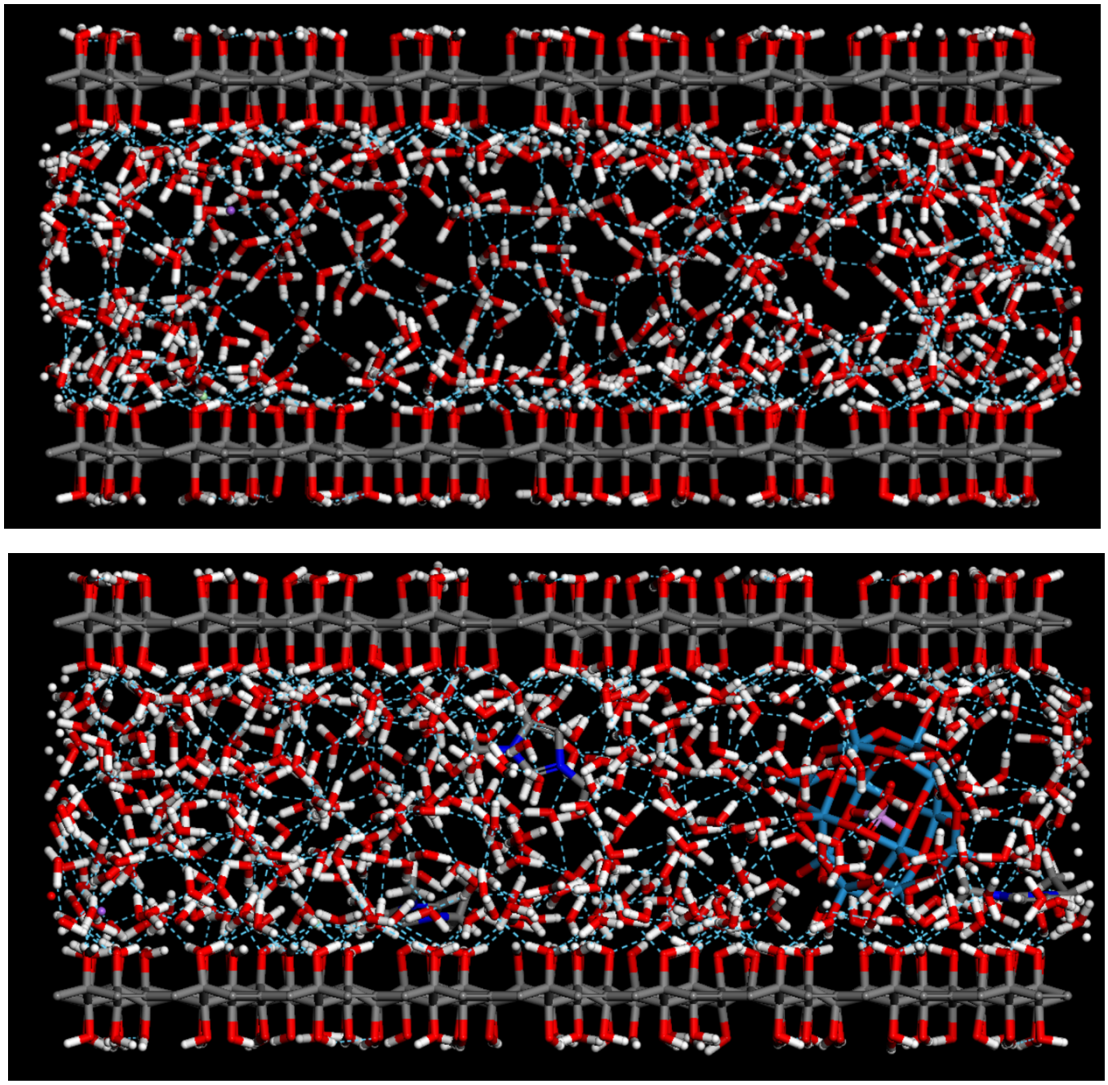


Fig. S2. The snapshots of the HBs (shown by dashed blue lines) for empty-GO and 1IL-GO systems. The HB cutoff distance (2.88 Å) and the HB angle of 150° were used as the criteria in this figure. The O, H, P, W, N, and C atoms are in red, white, pink, light blue, dark blue, and gray, respectively.