Electronic Supplementary Material

Molecular level understanding of CO_2 capture in ionic liquid/polyimide composite membrane

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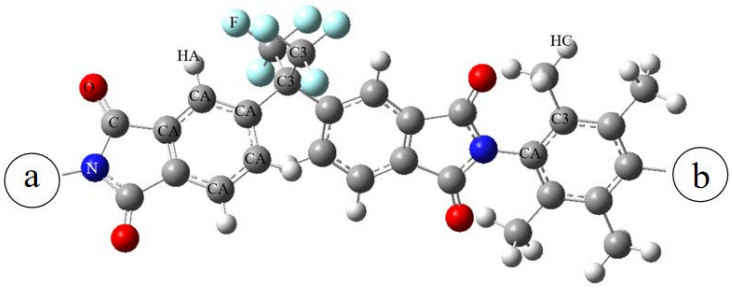
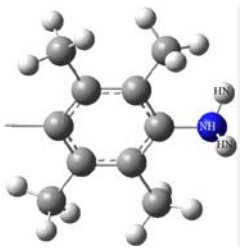
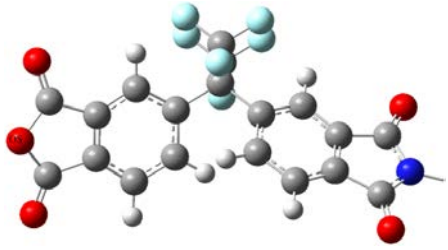


(a) The monomer of 6FDA-TeMPD PI



(b) The structure of a



(c) The structure of b

Figure S1 Schematic structure and atom type notations of 6FDA-TeMPD PI

Table S1. The force filed parameters for 6FDA-TeMPD PI

Non-bonded parameters

6FDA-TeMPD	σ ($\times 10^{-1}$ nm)	ε(kJ/mol)	source	q/e (ref 43)
CA	3.4	0.3598	GAFF	-0.4137
C3	3.4	0.4577	GAFF	-0.2926
HC	2.6	0.0657	GAFF	0.0876
N	3.3	0.7113	GAFF	0.3200
C	3.4	0.3598	GAFF	0.3900
O	3.0	0.8786	GAFF	-0.4192
HA	2.6	0.0628	GAFF	0.1224
F	3.1	0.2552	GAFF	-0.1014
OS	2.9	0.7113	GAFF	0.4159
HN	1.1	0.0569	GAFF	0.3490
NH	3.3	0.7113	GAFF	-0.8647

Bonded parameters 1 (bonds)

6FDA-TeMPD	r_0 ($\times 10^{-1}$ nm)	K_b ($\times 10^5$ kJ mol^{-1} nm^{-2})	function	source
CA-CA	1.40	3.86	1	GAFF
C-N	1.41	3.22	1	GAFF
C -CA	1.52	2.69	1	GAFF
C3-HC	1.10	2.77	1	GAFF
N-C3	1.38	3.58	1	GAFF
C -C	1.49	2.89	1	GAFF
CA-O	1.22	5.34	1	GAFF
CA-HC	1.09	2.89	1	GAFF
C-C	1.54	2.52	1	GAFF
C3-F	1.35	2.99	1	GAFF
CA -OS	1.36	3.27	1	GAFF
C-NH	1.39	3.50	1	GAFF
N-HN	1.01	3.39	1	GAFF

Bonded parameters 2 (angles)

6FDA-TeMPD	θ_0 (deg)	K_a (kJ mol^{-1} rad^{-2})	6FDA-TeMPD	θ_0 (deg)	K_a (kJ mol^{-1} rad^{-2})	function	source
CA-CA-C3	120	557	CA-C-CA	112	532	1	GAFF

CA-CA-C	121	531	CA-C-C	112	528	1	GAFF
CA-N-C	124	534	C-C-F	109	553	1	GAFF
CA-CA-CA	120	568	C-C-C	112	526	1	GAFF
CA-CA-HC	110	392	F-C-F	107	593	1	GAFF
HC-C-HC	108	330	C-CA-OS	112	580	1	GAFF
N-C-C	115	567	CA-OS-CA	121	534	1	GAFF
N-C-O	123	621	C-C-O	123	630	1	GAFF
C-N-C	127	533	CA-CA-NH	121	572	1	GAFF
CA-CA-C	120	538	CA-NH-H	116	405	1	GAFF
C-C-O	123	575	H-NH-H	115	336	1	GAFF
C-CA-HA	120	403				1	GAFF

Bonded parameters 3 (dihedrals)

6FDA-TeMPD	φ (deg)	K_i (kJ/mol)	function	source
	Proper Torsions			
CA- CA-CA-CA	180	15.17	9	GAFF
CA-CA-C3-HC	0	0	9	GAFF
CA-N-C-CA	180	10.46	9	GAFF
CA-CA-N- C	180	1.88	9	GAFF
N-C-CA-CA	180	4.18	9	GAFF
CA-C3-C3-F	0	0.65	9	GAFF
C-CA-OS-CA	180	11.30	9	GAFF
CA-CA-CA- H	180	4.39	9	GAFF
	Improper Torsions			
CA-CA-CA-C	180	4.60	2	GAFF
CA-N-C-O	180	43.93	2	GAFF

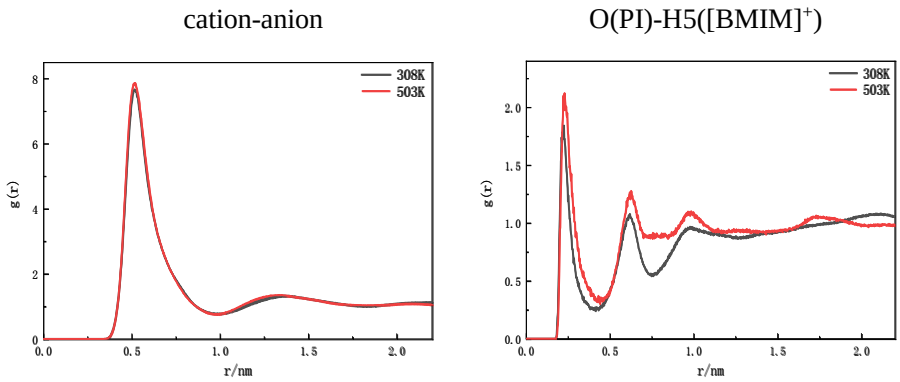
Table S2. The simulated density and experimental density for the mixture of [BMIM][Tf_2N] and 6FDA-TeMPD PI.

	[a]Simulated density (g/cm^3)	[b]Experimental density (g/cm^3)
PI	1.167	1.323±0.029
10wt%IL	1.224	1.332±0.003
20wt% IL	1.294	-

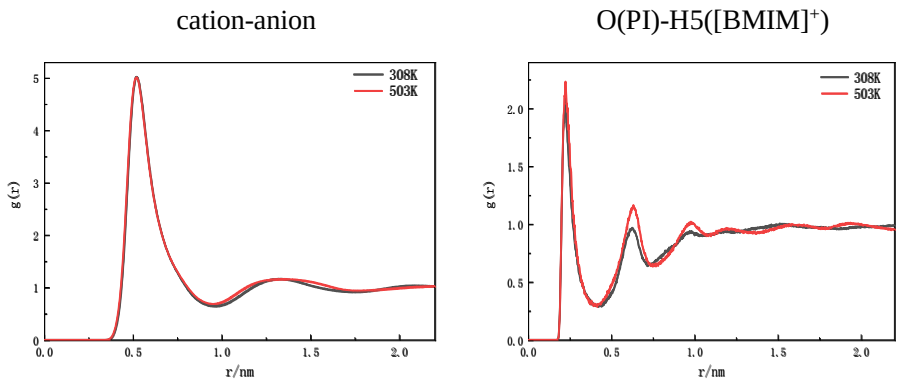
30wt% IL	1.354	-
35wt% IL	1.364	1.353±0.024
40wt% IL	1.395	-
50wt% IL	1.430	1.382±0.014
Pure IL	1.550	1.440

[a] Density at 308 K. [b]Experimental densities measured at 308 K were obtained from Ref 15.

(a) 20 wt%IL



(b) 35 wt%IL



(c) 50 wt%IL

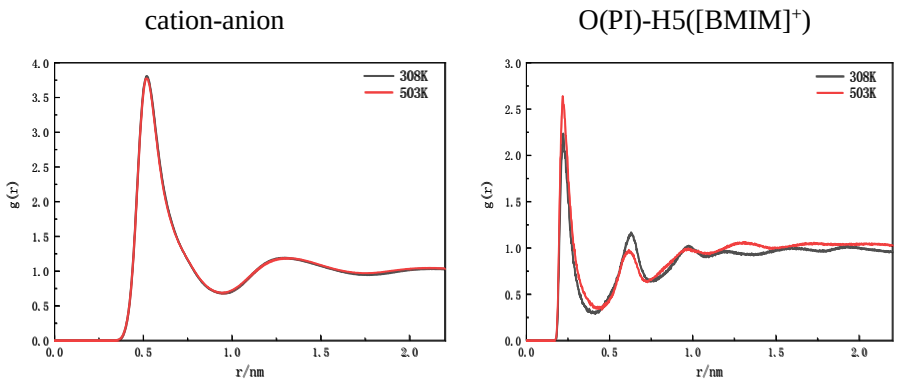


Figure S2. Center-of-mass RDFs of cation-anion, and site-site RDFs for H5 atoms in cations and O atoms in PI with (a) 20wt%IL, (b)35wt%IL, and (c) 50wt%IL.

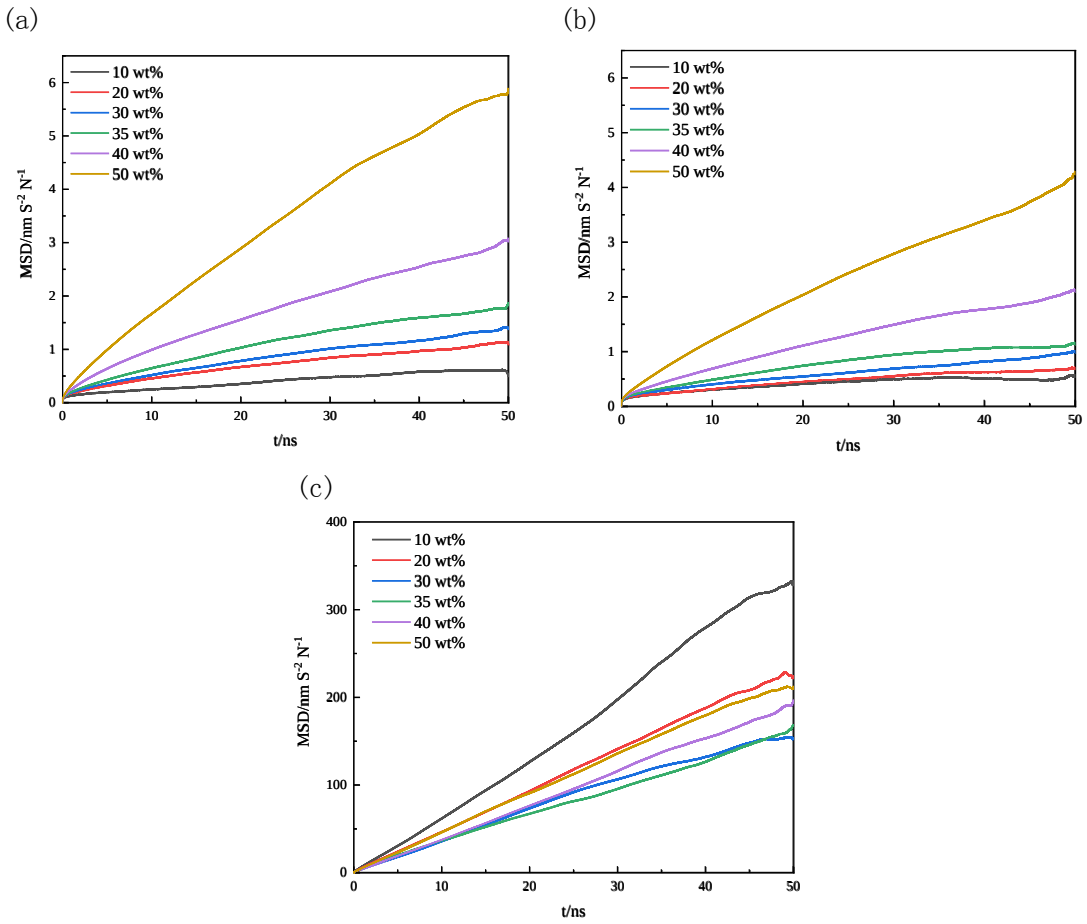
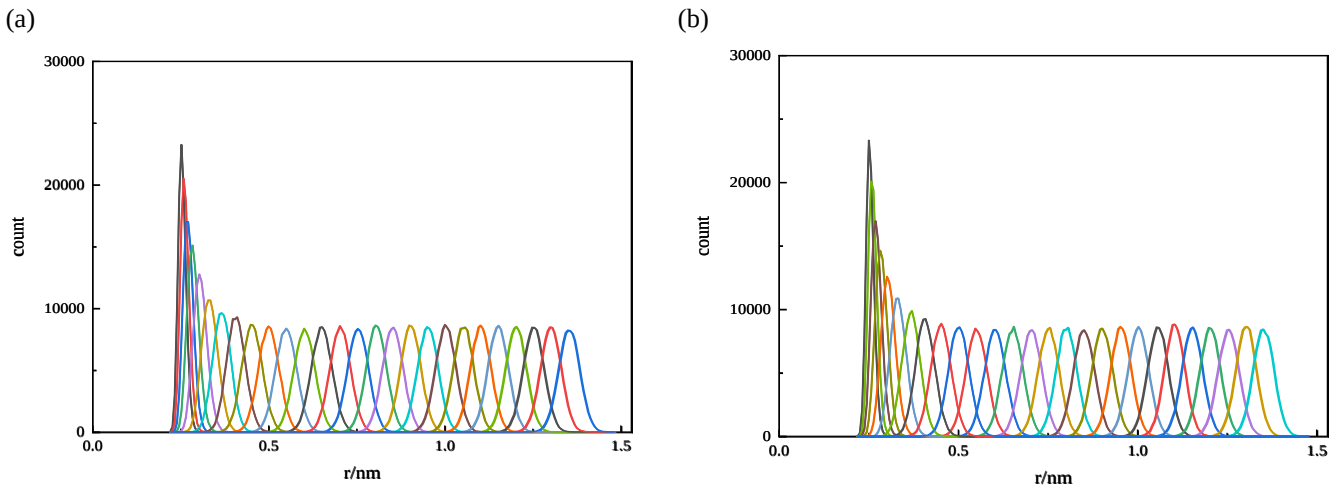


Figure S3. The mean square displacement curves of (a) $[BMIM]^+$, (b) $[Tf_2N)]^-$, (c) CO_2 with different IL concentrations.



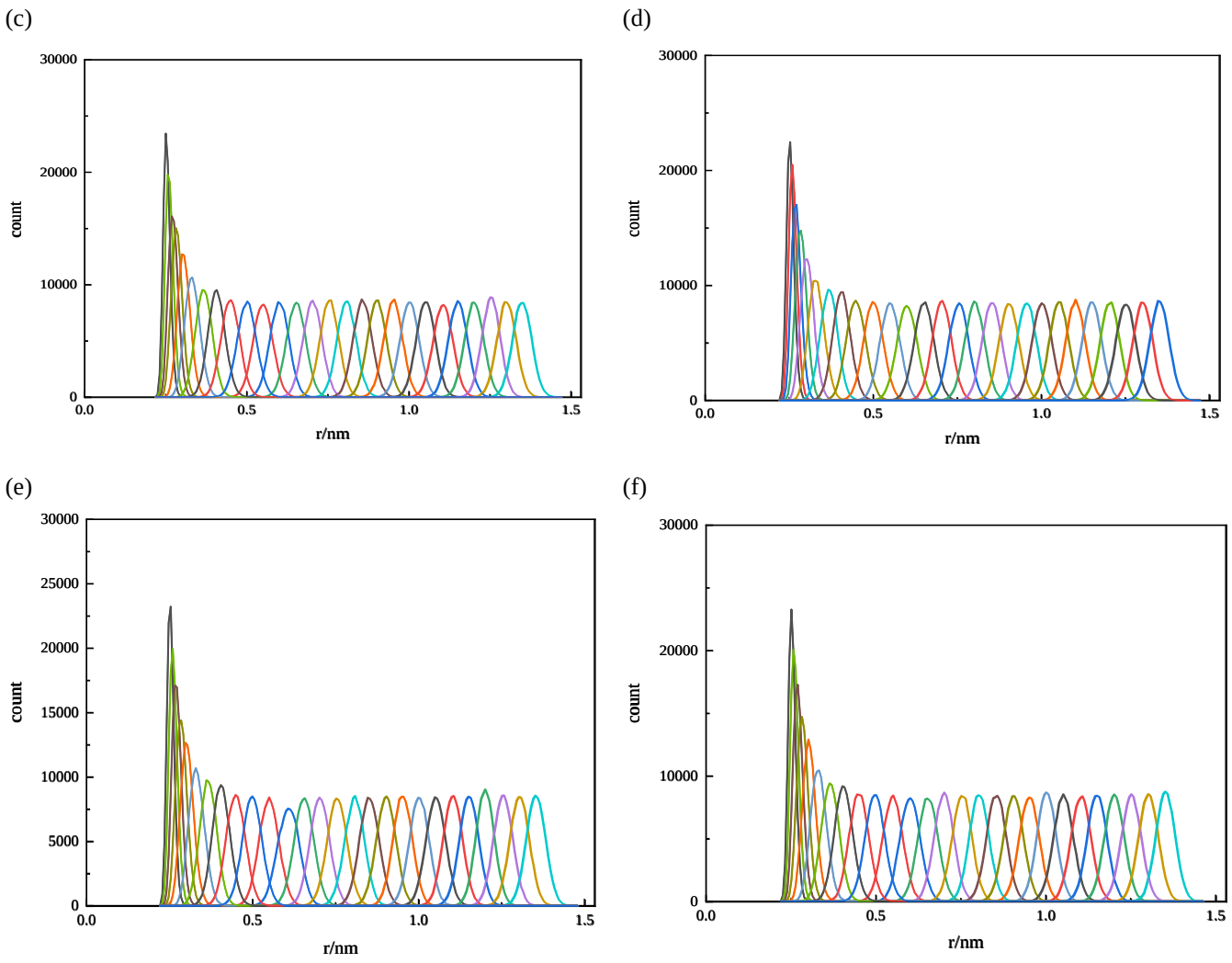


Figure S4. The histogram of calculated PMF of CO_2 with (a) 10 wt% IL, (b) 20 wt% IL, (c) 30 wt% IL, (d) 35 wt% IL, (e) 40 wt% IL, and (f) 50 wt% at 503 K and 1bar.