

Electronic Supplementary Information

Metal-Organic Framework Supported Ionic Liquid Membranes for CO₂ Capture: Anion Effects

Krishna M. Gupta, Yifei Chen, Zhongqiao Hu and Jianwen Jiang*

Department of Chemical and Biomolecular Engineering, National University of Singapore, 117576, Singapore

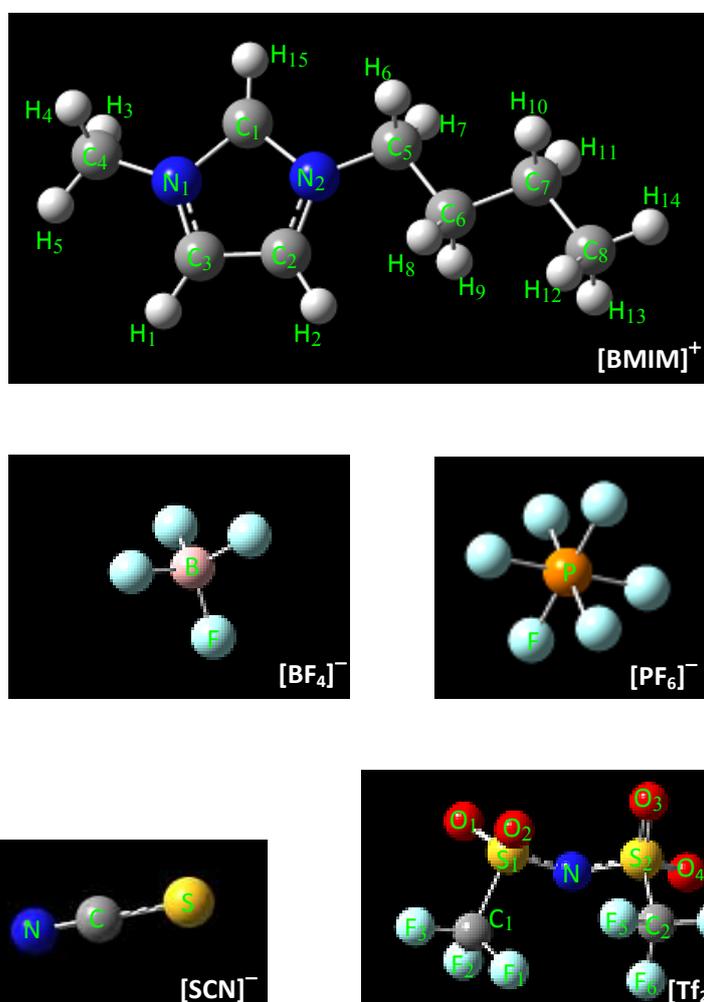


Figure S1. Atomic types in [BMIM]⁺, [BF₄]⁻, [PF₆]⁻, [SCN]⁻, and [Tf₂N]⁻.

Table S1. Atomic charges in [BMIM]⁺, [BF₄]⁻, [PF₆]⁻, [SCN]⁻, and [Tf₂N]⁻.

[BMIM]⁺

Atom	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	C ₈	N ₁	N ₂
Charge	-0.158	-0.151	-0.236	-0.316	-0.342	0.136	0.112	-0.315	0.218	0.276
Atom	H ₁	H ₂	H ₃	H ₄	H ₅	H ₆	H ₇	H ₈	H ₉	H ₁₀
Charge	0.205	0.251	0.162	0.164	0.170	0.143	0.145	0.009	0.009	0.009
Atom	H ₁₁	H ₁₂	H ₁₃	H ₁₄	H ₁₅					
Charge	0.008	0.082	0.111	0.079	0.230					

[BF₄]⁻

Atom	B	F
Charge	1.134	-0.533

[PF₆]⁻

Atom	P	F
Charge	1.34	-0.39

[SCN]⁻

Atom	S	C	N
Charge	-0.722	0.459	-0.737

[Tf₂N]⁻

Atom	N	S ₁	S ₂	C ₁	C ₂	O ₁	O ₂	O ₃	O ₄
Charge	-0.670	1.093	1.031	0.389	0.235	-0.552	-0.524	-0.545	-0.549
Atom	F ₁	F ₂	F ₃	F ₄	F ₅	F ₆			
Charge	-0.150	-0.192	-0.168	-0.145	-0.133	-0.118			

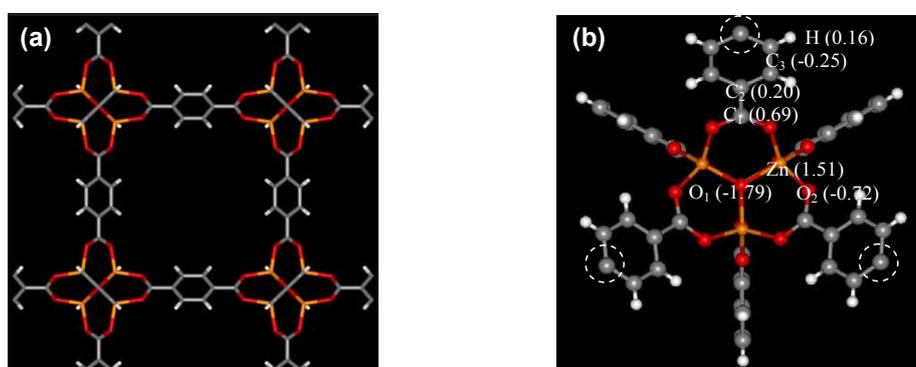


Figure S2. (a) IRMOF-1 structure. (b) Atomic types and charges. Color code: Zn, orange; O, red; C, grey; H, white.

Table S2. Densities (kg/m^3) of ILs from simulation and experiment at 1 atm and different temperatures.

[BMIM][BF ₄]		
<i>T</i> (°C)	Simulation	Experiment ¹
30	1190	1200
50	1185	1194
60	1174	1185
70	1162	1173
[BMIM][Tf ₂ N]		
<i>T</i> (°C)	Simulation	Experiment ¹
23	1495	1439
40	1485	1434
50	1474	1425
60	1464	1414
[BMIM][PF ₆]		
<i>T</i> (°C)	Simulation	Experiment ²
20	1354	1360
40	1344	1348
50	1337	1340
60	1328	1332
70	1320	1324
[BMIM][SCN]		
<i>T</i> (°C)	Simulation	Experiment ³
20	1103	1070
45	1090	1058
55	1085	1052
65	1079	1046
75	1073	1041

1. C. P. Fredlake, J. M. Crosthwaite, D. G. Hert, S. N. V. K. Aki and J. F. Brennecke, *J. Chem. Eng. Data*, 2004, **49**, 954-964.
2. Z. Y. Gu and J. F. Brennecke, *J. Chem. Eng. Data*, 2002, **47**, 339-345.
3. U. Domanska and M. Krolikowska, *J. Chem. Eng. Data*, 2010, **55**, 2994-3004.

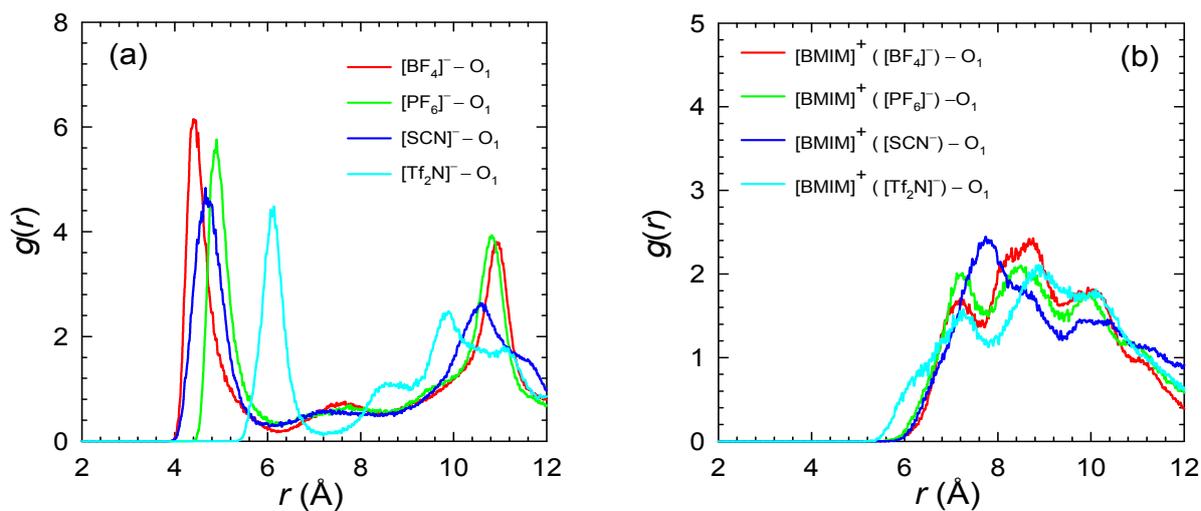


Figure S3. Radial distribution functions of (a) anion (b) cation around O_1 atom of IRMOF-1 in IL/IRMOF-1 membranes at $W_{IL/IRMOF-1} = 0.4$.

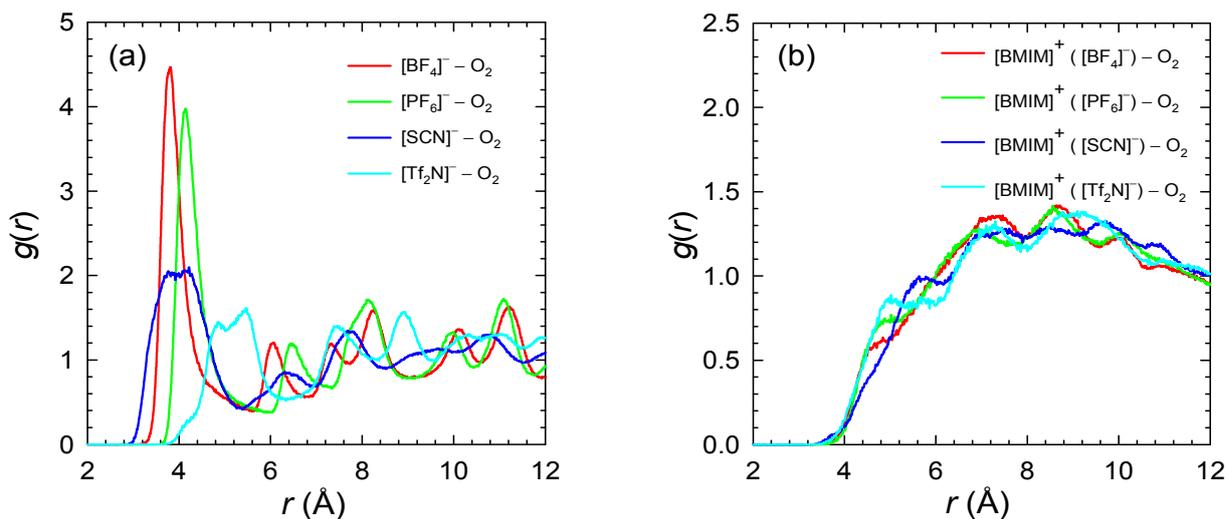


Figure S4. Radial distribution functions of (a) anion (b) cation around O_2 atom of IRMOF-1 in IL/IRMOF-1 membranes at $W_{IL/IRMOF-1} = 0.4$.

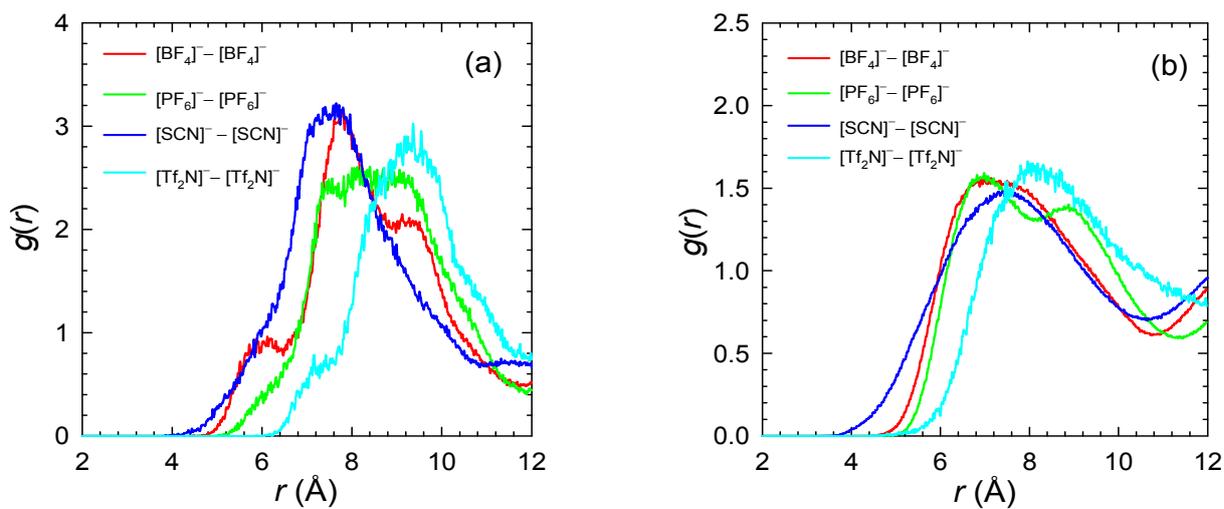


Figure S5. Radial distribution functions of anion-anion in (a) IL/IRMOF-1 membranes at $W_{IL/IRMOF-1} = 0.4$ (b) bulk phase.

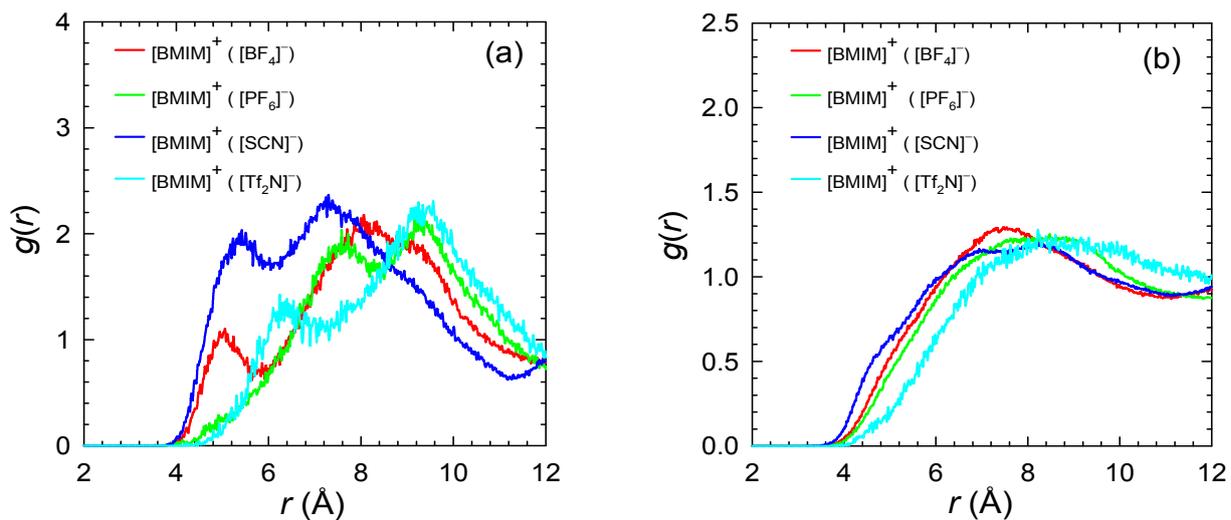


Figure S6. Radial distribution functions of cation-cation of ILs in (a) IL/IRMOF-1 membranes at $W_{IL/IRMOF-1} = 0.4$ (b) bulk phase.