Electronic Supplementary Information

CO_2 capture in poly(ionic liquid) membranes: atomistic insight into the role of anions

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Table S1 Atomic charges in $[VBIM]^+$. The C8 and C9 atoms are the head and tail to form polymeric $[VBIM]^+$ chain.

Atom	C1	C2	C3	C4	C5	C6	C7	C8	C9
Charge	-0.455	0.008	0.016	-0.416	-0.263	-0.128	-0.268	-0.084	-0.254
Atom	H1	H2	H3	H4	H5	H6	H7	H8	H9
Charge	0.155	0.120	0.133	0.065	0.062	0.067	0.071	0.182	0.185
Atom	H10	H11	H12	H13	H14	H15	N1	N2	
Charge	0.290	0.210	0.290	0.156	0.181	0.172	0.247	0.258	

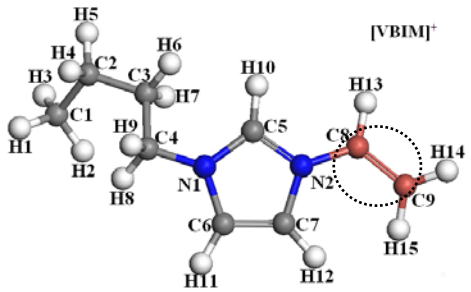

Table S2 Atomic charges in $[TF_2N]^-$.

Atom	C1	C2	S1	S2	O1	O2	O3	O4
Charge	0.268	0.219	0.721	0.773	-0.395	-0.444	-0.438	-0.400
Atom	N	F1	F2	F3	F4	F5	F6	
Charge	-0.569	-0.130	-0.123	-0.121	-0.126	-0.088	-0.147	

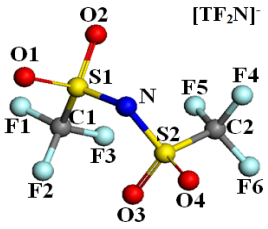

Table S3 Atomic charges in $[SCN]^-$.

Atom	C	N	S
Charge	0.459	-0.737	-0.722

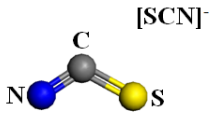

Table S4 Atomic charges in $[PF_6]^-$.

Atom	P	F
Charge	1.34	-0.39

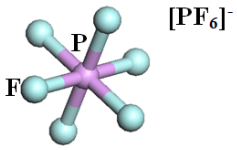

Table S5 Atomic charge in $[Cl]^-$.

Atom	Cl
Charge	-1.00

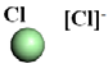

Table S6 Atomic charges in $[BMIM]^+$.

Atom	C1	C2	C3	C4	C5	C6	C7	C8	N1	N2
Charge	-0.486	0.048	0.027	-0.392	-0.257	-0.200	-0.224	-0.463	0.280	0.232
Atom	H1	H2	H3	H4	H5	H6	H7	H8	H9	H10
Charge	0.130	0.159	0.135	0.053	0.052	0.066	0.055	0.172	0.178	0.286
Atom	H11	H12	H13	H14	H15					
Charge	0.242	0.273	0.213	0.208	0.213					

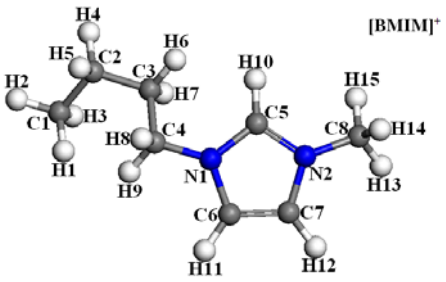

Table S7 Densities (g/cm^3) of $[BMIM][TF_2N]$ and [BMIM][SCN] at 300 K and 1 atm.

IL	Sim.	Exp.
$[BMIM][TF_2N]$	1.476 ± 0.004	1.430,[1] 1.434,[2] 1.436[2]
[BMIM][SCN]	1.040 ± 0.002	1.070[3]

Table S8 Solubility parameters δ $[(J/cm^3)^{0.5}]$ and vaporization enthalpies ΔH^{vap} [kJ/mol] of $[BMIM][TF_2N]$ and [BMIM][SCN] at 300 K and 1 atm.

IL	Solubility Parameter δ		ΔH^{vap}	
	Exp.	Sim.	Exp.	Sim.
$[BMIM][TF_2N]$	19.8[4], 20.9[5], 21.2[6], 25.5[7], 26.7[8]	24.5	134.0[6], 191.0[7], 208.2[8]	174.3
[BMIM][SCN]	24.6[9]	30.4	–	175.9

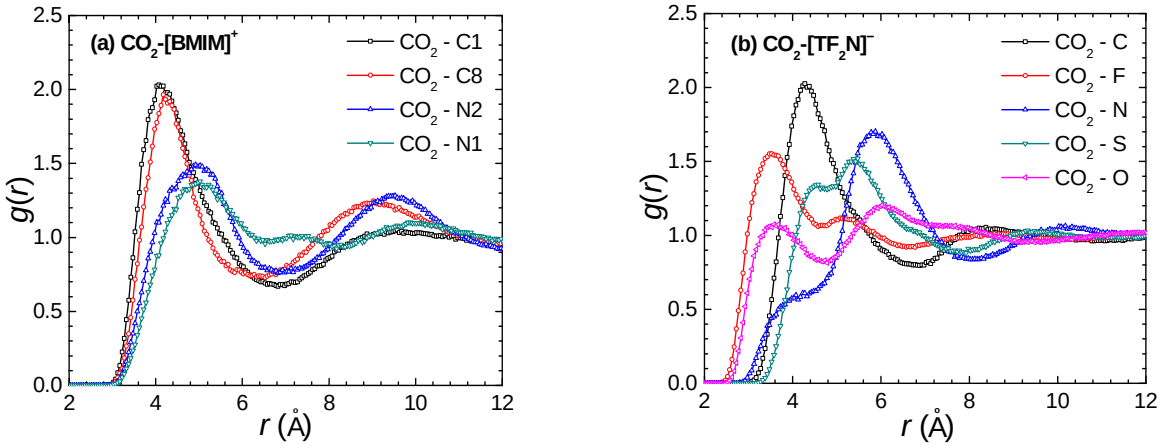

Fig. S1 Radial distribution functions of CO_2 in [BMIM][TF_2N].
(a) CO_2-$[BMIM]^+$ (b) CO_2-$[TF_2N]^-$.

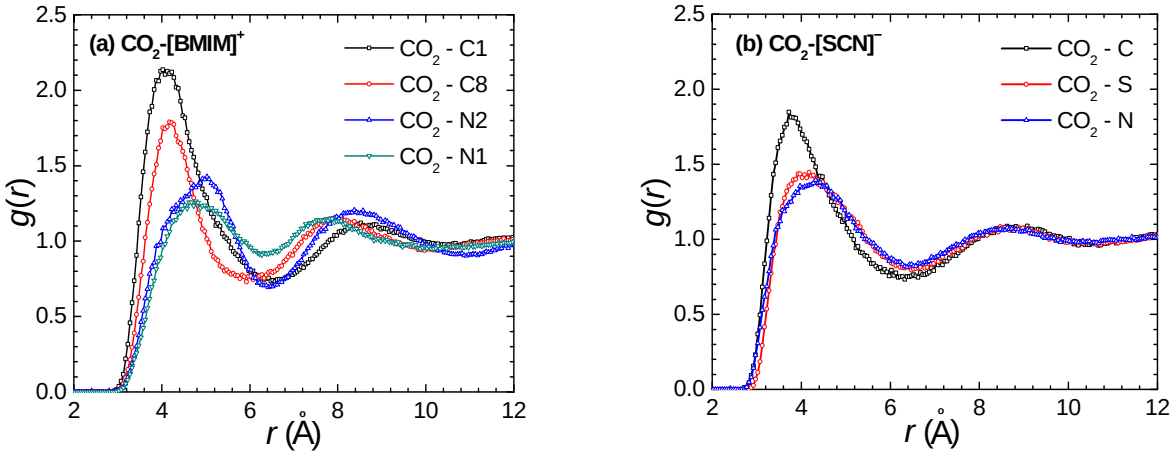

Fig. S2 Radial distribution functions of CO_2 in [BMIM][SCN].
(a) CO_2-$[BMIM]^+$ (b) CO_2-$[SCN]^-$.

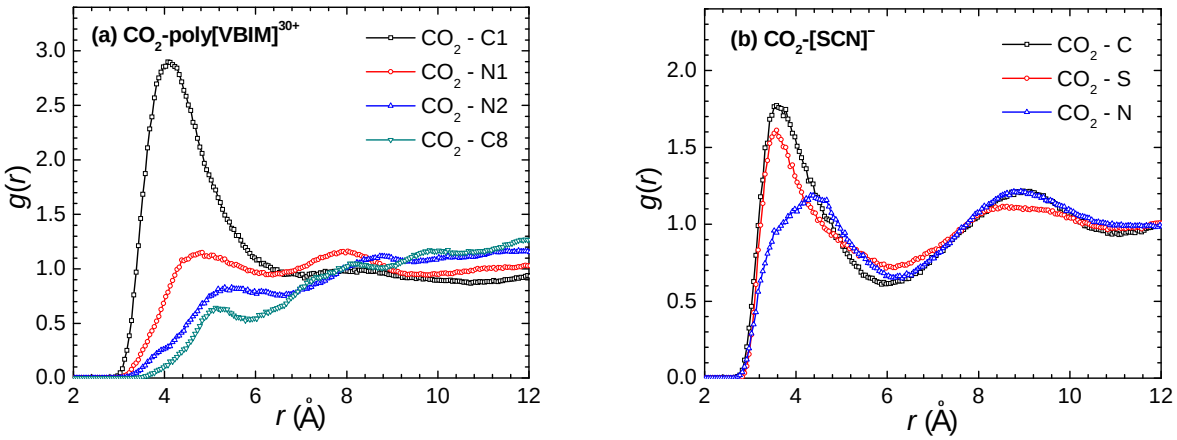

Fig. S3 Radial distribution functions of CO_2 in poly([VBIM][SCN]). (a) CO_2-poly[VBIM]$^{30+}$ (b) CO_2-$[SCN]^-$.

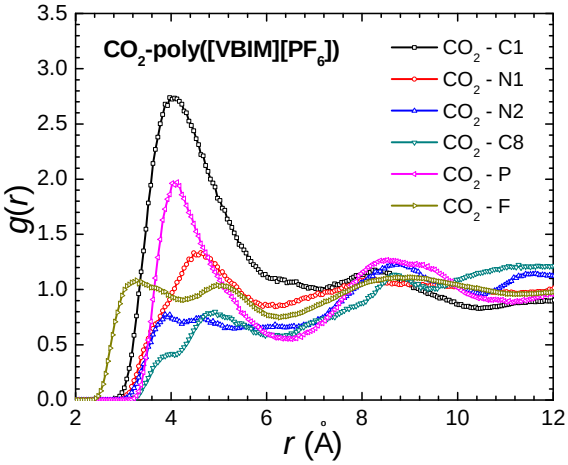

Fig. S4 Radial distribution functions of CO_2 in poly([VBIM][PF_6]).

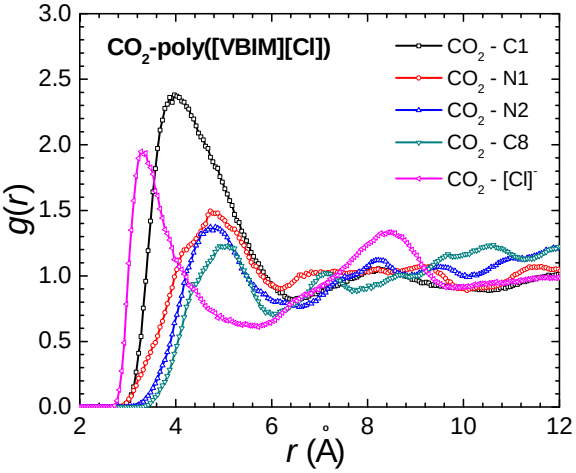

Fig. S5 Radial distribution functions of CO_2 in poly([VBIM][Cl]).

References

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