Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for

Molecular mechanism of CO_2 absorption in Phosphonium Amino Acid Ionic Liquid

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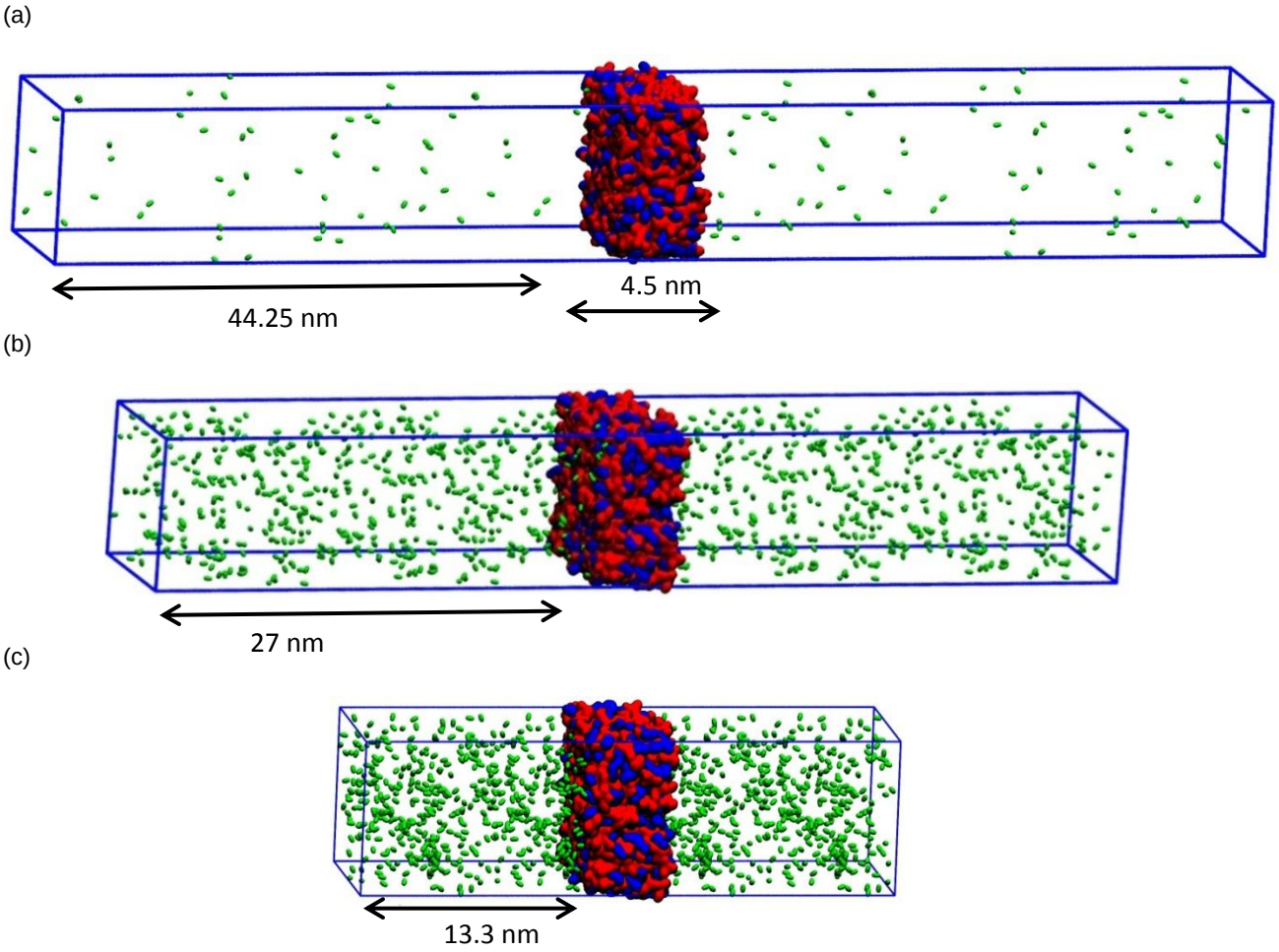


Figure S1. Initial configuration of CO_2-IL slabs at (a) 1 bar, (b) 10 bar and (c) 20 bar partial pressure of CO_2. Box dimensions (in nm) are (a) 4.5 x 4.5 x 92.0, 128:512 CO_2-IL molecules (b) 4.5 x 4.5 x 58.4, 1024:512 CO_2-IL molecules and (c) 4.5 x 4.5 x 31.1, 1024:512 CO_2-IL molecules.

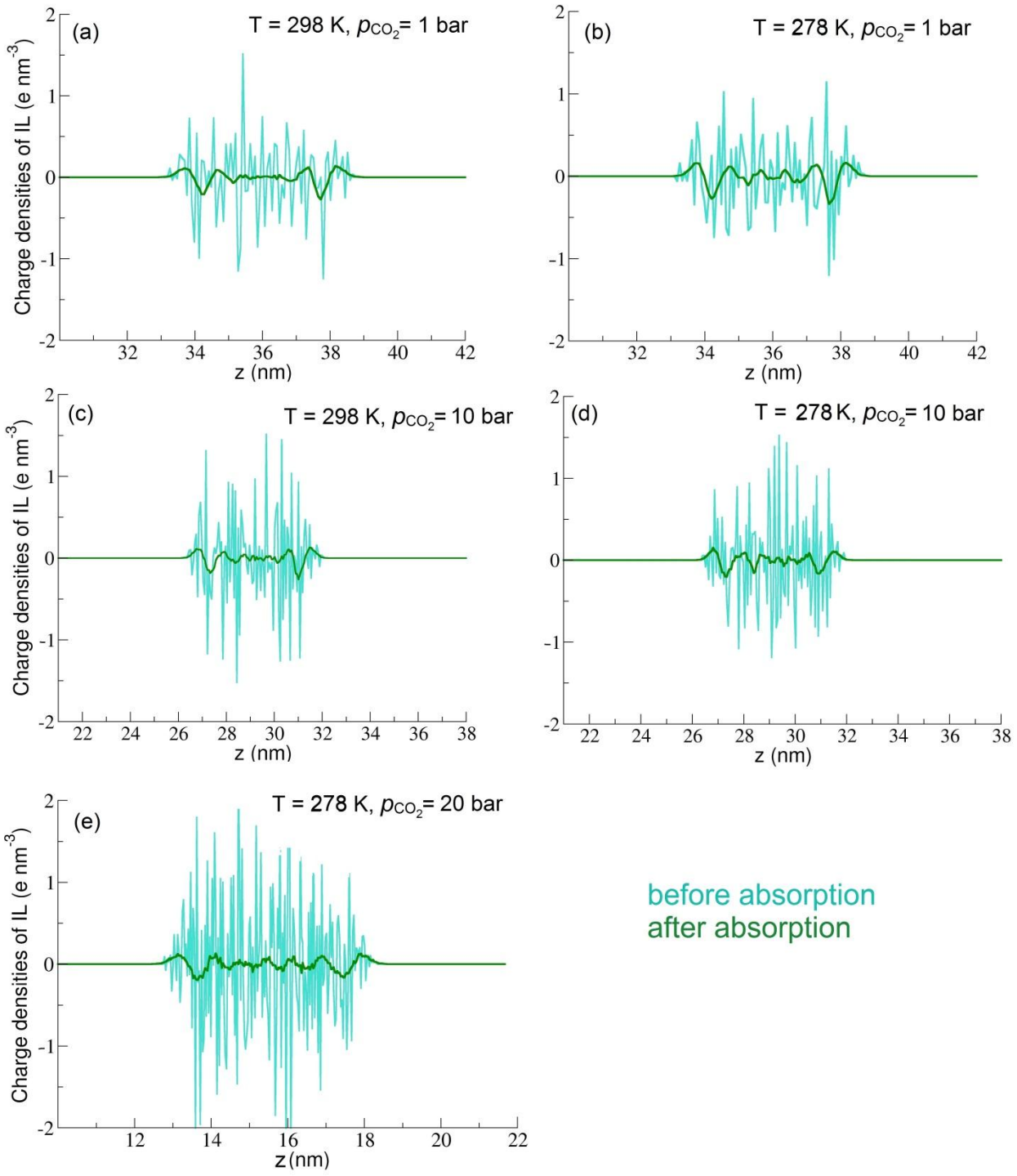


Figure S2. Charge densities of IL before and after absorption of CO_2 at different thermodynamic conditions.

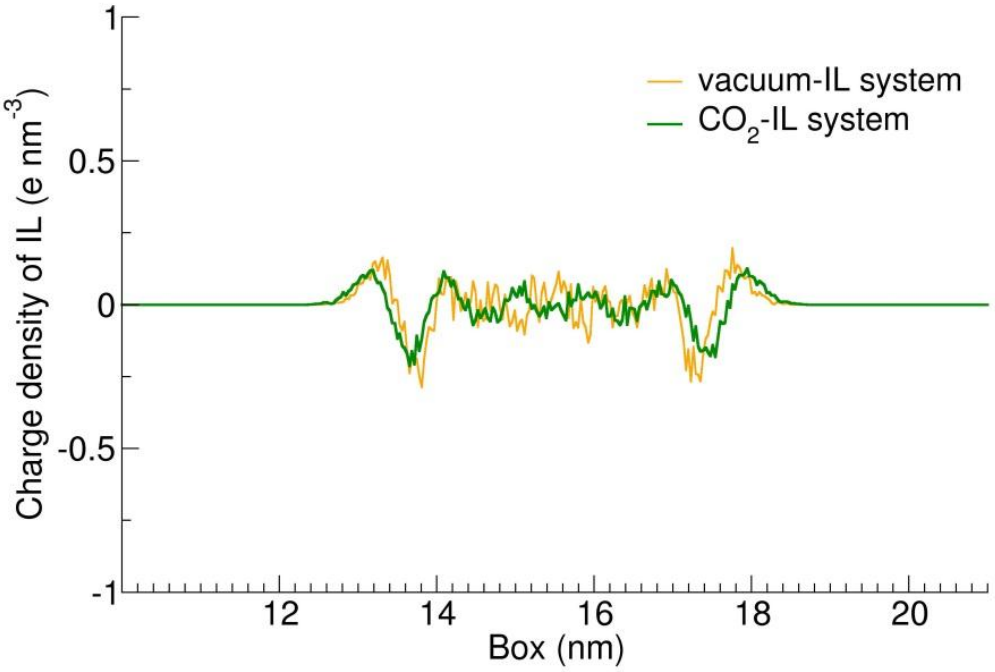


Figure S3. Averaged charge densities (from t = 5 ns to t = 10 ns) of IL for vacuum *vs* CO_2 in IL system, both at T = 298 K, and for CO_2-IL system p_{CO_2} = 20 bar.

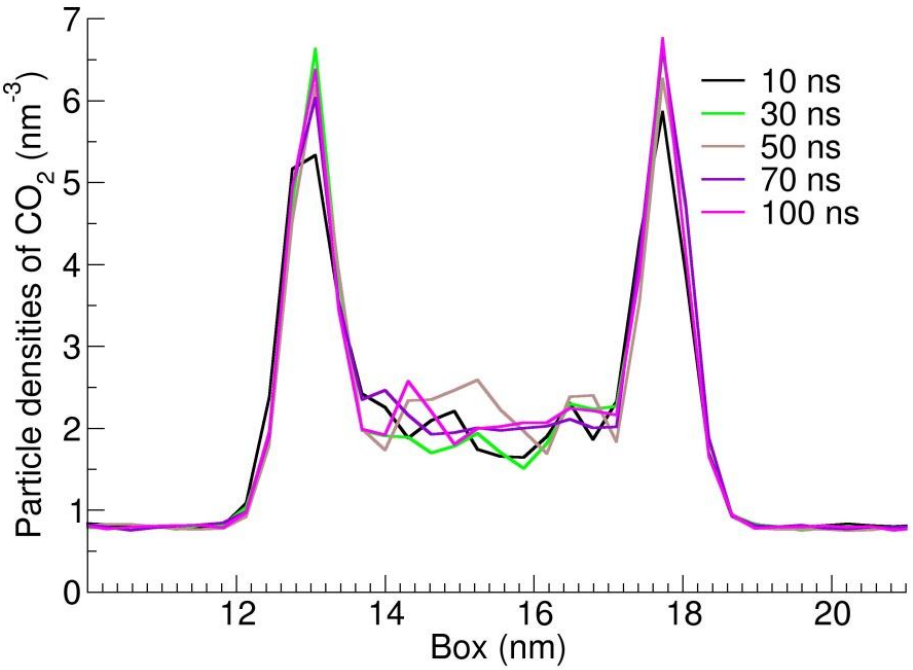


Figure S4. Particle densities of CO_2 in CO_2-IL interface at T = 298 K, p_{CO_2} = 20 bar.

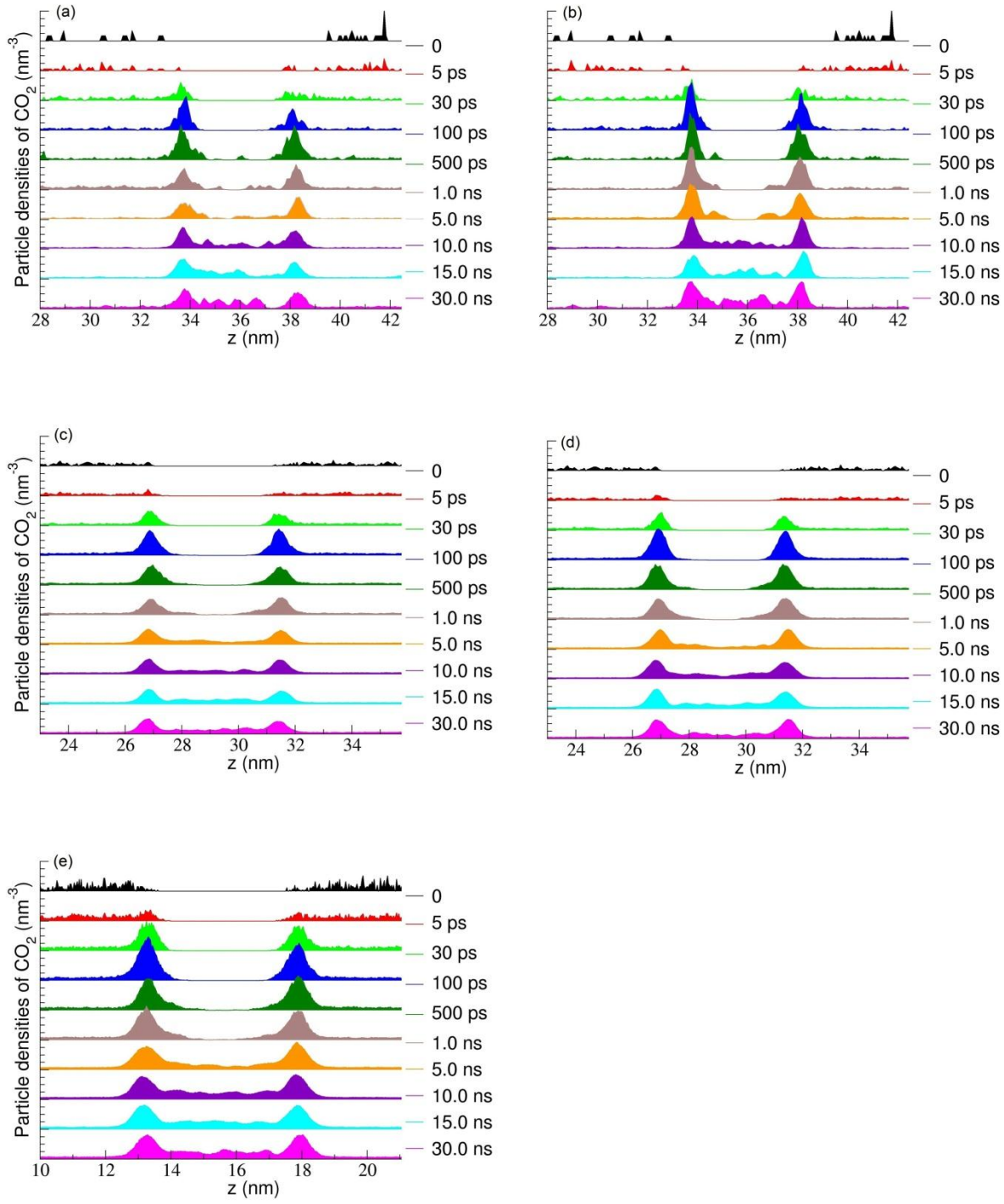


Figure S5. Particle densities of CO_2 at respective T and p_{CO_2}, (a) 298 K, 1 bar; (b) 278 K, 1 bar; (c) 298 K, 10 bar; (d) 278 K, 10 bar; (e) 278 K, 20 bar. In the y – axis, each minor tick corresponds to a value of 0.25 particle nm^{-3} for (a) and (b), and 2.5 particle nm^{-3} for (c), (d) and (e).

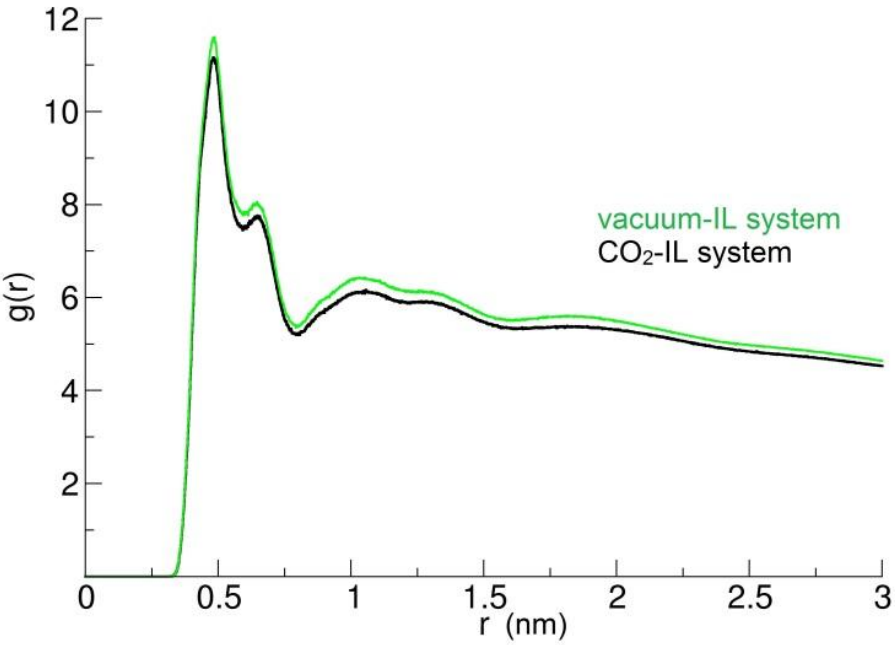


Figure S6. Averaged site-site RDF (t = 25 ns to t = 35 ns) between P[P_{4444}]-N1,N2[Lys] for CO_2-IL interface(black) and for vacuum-IL interface(green) at T = 298 K and p_{CO_2}= 20 bar.

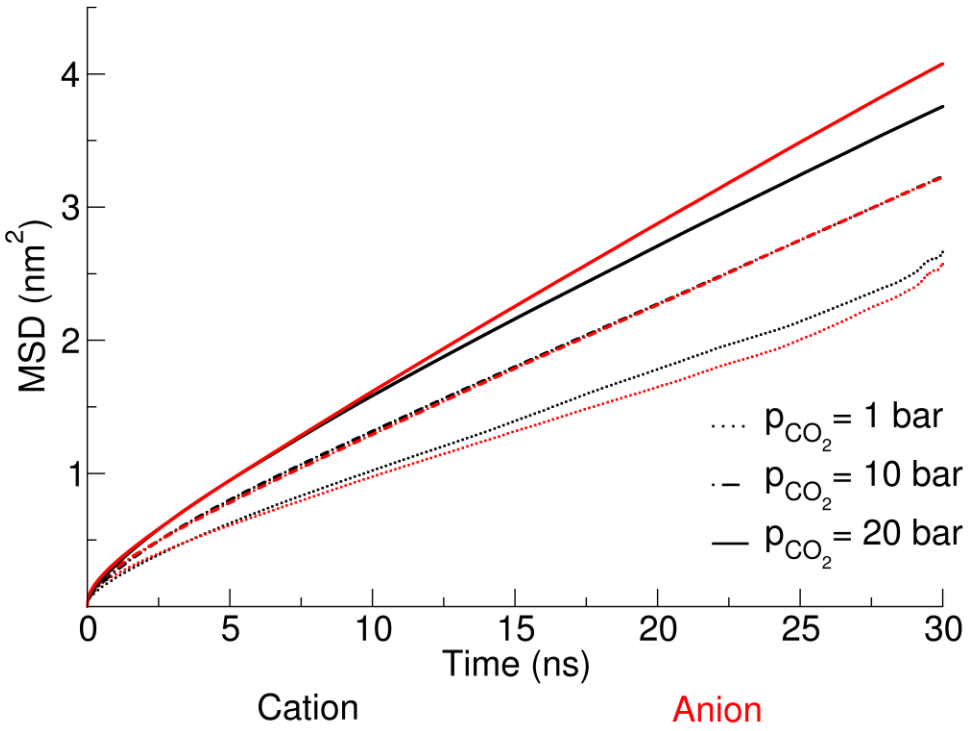
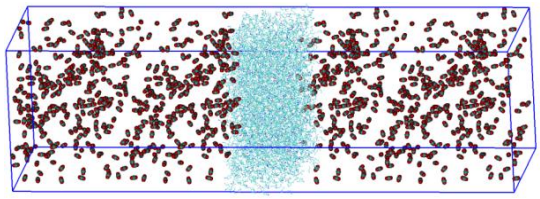
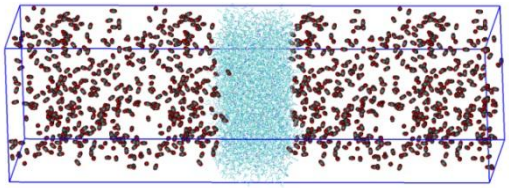


Figure S7. MSDs of cations and anions of IL at T = 298 K.



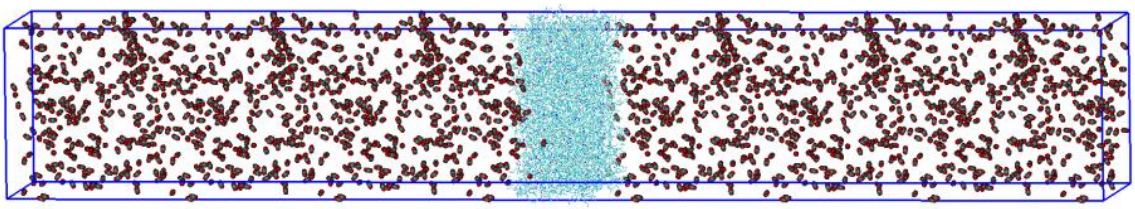
1024 CO_2 : 512 IL

(a)



1024 CO_2 : 512 IL

(b)



2048 CO_2 : 512 IL

(c)

Figure S8. Initial configurations of CO_2-IL system at p_{CO_2}= 20 bar and T = 298 K: Configurations (a) and (b) differ in positions and configuration (c) differ in system size.

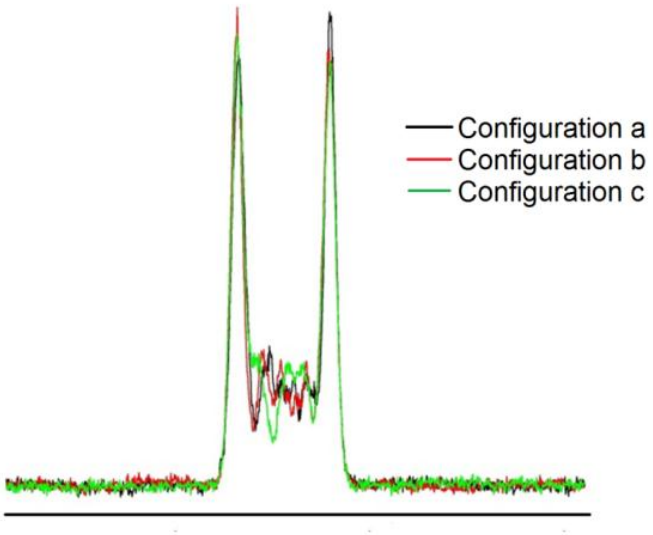


Figure S9. Averaged particle densities of CO_2 inside the box (t = 25 ns to t = 35 ns) for the CO_2-IL system.

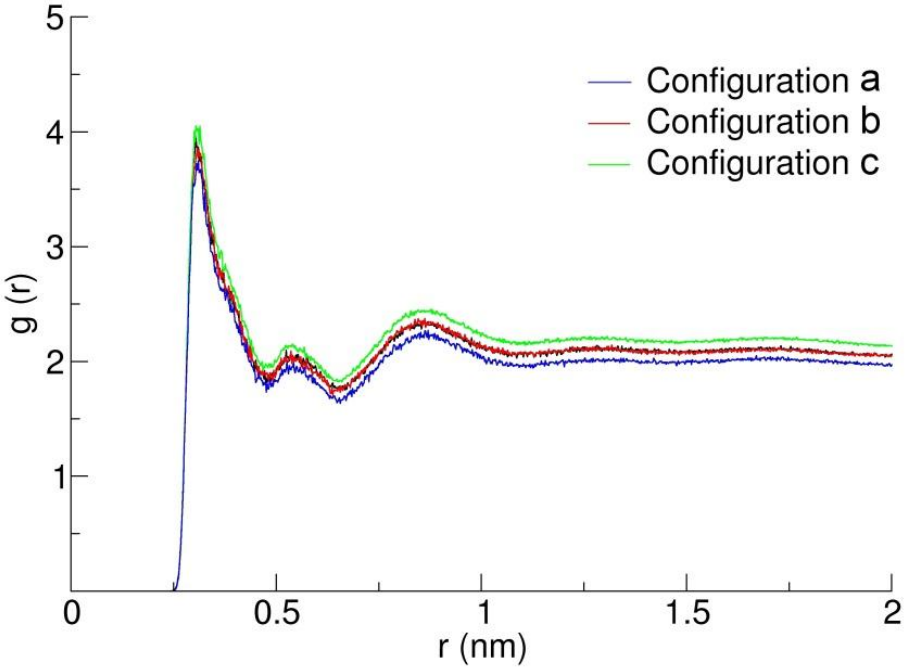


Figure S10. Averaged site-site RDFs (t = 25 ns to t = 35 ns) between N1,N2[Lys]-C[CO_2] at p_{CO_2}= 20 bar and T = 298 K.

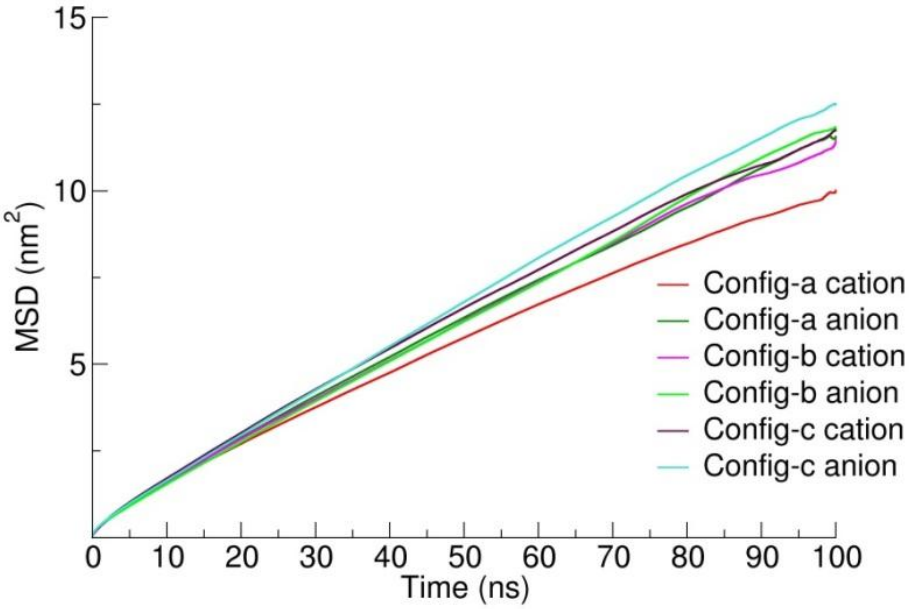


Figure S11. MSDs of [P_{4444}] and [Lys] at p_{CO_2} = 20 bar and T = 298 K.

Table S1. Standardization of force field for IL with experiment and simulation

Properties	**Previous work**	**Our work**
Density at 298.15 K (g/cm^3)	0.973 *	0.963
	0.962 **	
Density at 321.85 K (g/cm^3)	0.950 **	0.945
CoM RDF between Cation and anion (298.15 K)		
First Maxima (Å)	5.85 **	6.05
First Minima (Å)	8.05 **	8.21
Peak height	2.28 **	2.32
Coordination number	3.55 **	3.75
Conductivity of anion (S/cm)	0.83 x 10^{-4} *	0.78 x 10^{-4}

* G. Zhou, X. Liu, S. Zhang, G. Yu and H. He, *J. Phys. Chem. B*, 2007, **111**, 7078–7084.

** (a) Zhang, J. M.; Zhang, S. J.; Dong, K.; Zhang, Y. Q.; Shen, Y.; Lu, X. *Chem. Eur. J*, 2006, **12,** 4021–4026. (b) Zhang, J. M.; Zhang, S. J. Combinatorial chemistry research on amino acids and ionic liquids. Postdoctoral Thesis, Institute of Process Engineering, Chinese Academy of Sciences, 2005.

Table S2. Molar absorption ratio (calculated as an average from *t* = 10.0 ns to *t* = 30.0 ns) at various thermodynamic conditions

Total no. of CO_2 molecules	Temperature (K)	p_{CO_2} (bar)	No. of CO_2 molecules absorbed	Molar absorption ratio CO_2:IL
128	298	1.0	36	0.070
128	278	1.0	49	0.096
1024	298	10.0	308	0.602
1024	278	10.0	358	0.699
1024	298	20.0	469	0.916
1024	278	20.0	553	1.080