Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary material

Carbon dioxide capture by aminoalkyl imidazolium-based ionic liquid: A computational investigation

Jie-Jie Chen[1], Wen-Wei Li[1], Xue-Liang Li[2,]*, Han-Qing Yu[1,]*

[1]Department of Chemistry, University of Science & Technology of China, Hefei, 230026, China

[2]School of Chemical Engineering, Hefei University of Technology, Hefei, 230009, China

***Corresponding authors:**

Prof. Xue-Liang Li, E-mail: lixuel987@163.com;

Prof. Han-Qing Yu, E-mail: hqyu@ustc.edu.cn

The following is included as additional supporting materials for this paper:

Table S1 Thermodynamic parameters of Step 2 at ambient temperature (298.15 K) and atmosphere pressure (1 atm), including changes of standard Gibbs free energy (ΔG_2^{Θ}), enthalpy (ΔH_2^{Θ}) and entropy (ΔS_2^{Θ})

System	ΔG_2^{Θ} (kJ/mol)	ΔH_2^{Θ} (kJ/mol)	ΔS_2^{Θ} (J/mol·K)
[ammim]BF_4	109.35	162.27	177.52
[aemim]BF_4	148.30	212.91	216.73
[apmim]BF_4	128.18	196.71	229.84
[abmim]BF_4	40.69	122.70	275.03
[aamim]BF_4	48.97	97.88	164.06
[ahmim]BF_4	10.44	94.50	281.94

Table S2 Kinetic properties of Step 1 for AIILs capturing CO_2 at ambient temperature (298.15 K) and atmosphere pressure (1 atm), including activation energy (E_a), standard thermodynamic properties of activation ($\Delta^{\neq}G^{\Theta}$, $\Delta^{\neq}H^{\Theta}$, $\Delta^{\neq}S^{\Theta}$) and rate constants of absorption reaction (k)

System	E_a (kJ/mol)	$\Delta^{\neq}G^{\Theta}$ (kJ/mol)	$\Delta^{\neq}H^{\Theta}$ (kJ/mol)	$\Delta^{\neq}S^{\Theta}$ (J/mol·K)	k (mol^{1-n}/L^{1-n}·s)
[ammim]BF_4	97.136	6.62	-108.45	-385.96	1.12×10^{-24}
[aemim]BF_4	146.892	11.05	-117.32	-430.55	1.00×10^{-35}
[apmim]BF_4	166.795	81.76	-71.36	-513.56	1.51×10^{-43}
[abmim]BF_4	28.150	92.17	-28.82	-405.79	1.26×10^{-13}
[aamim]BF_4	189.100	7.43	-106.88	-383.38	1.18×10^{-40}
[ahmim]BF_4	74.412	-42.47	-208.56	-557.06	1.23×10^{-29}

Table S3 Diffusion coefficient (*D*) of cations, anions and CO_2 in the AIIL-CO_2 systems at ambient temperature (298 K) and atmosphere pressure (1 atm)

System		Linear regression equation	R^2	*D* (10^{-7} cm^2/s)
[ammim]BF_4	Cation	y = 0.0072x + 0.5678	0.9315	1.2
	Anion	y = 0.0126x + 0.5676	0.9818	2.1
	CO_2	y = 0.0396x + 0.8153	0.9881	6.6
[aemim]BF_4	Cation	y = 0.0255x + 0.4386	0.9777	4.2
	Anion	y = 0.0259x + 0.9606	0.9797	4.3
	CO_2	y = 0.0916x + 1.5011	0.9838	15.3
[apmim]BF_4	Cation	y = 0.0283x + 0.2582	0.9966	4.7
	Anion	y = 0.0228x + 0.6409	0.9880	3.8
	CO_2	y = 0.0620x + 1.8432	0.9821	10.3
[abmim]BF_4	Cation	y = 0.0203x + 0.2571	0.9945	3.4
	Anion	y = 0.0230x + 0.5565	0.9892	3.8
	CO_2	y = 0.0710x + 0.5188	0.9839	11.8
[aamim]BF_4	Cation	y = 0.0119x + 0.3201	0.9541	2.0
	Anion	y = 0.0168x + 0.5092	0.9498	2.8
	CO_2	y = 0.0450x + 1.6793	0.9832	7.5
[ahmim]BF_4	Cation	y = 0.0107x + 0.5559	0.9517	1.8
	Anion	y = 0.0168x + 0.8253	0.9596	2.8
	CO_2	y = 0.0276x + 1.3549	0.9216	4.6

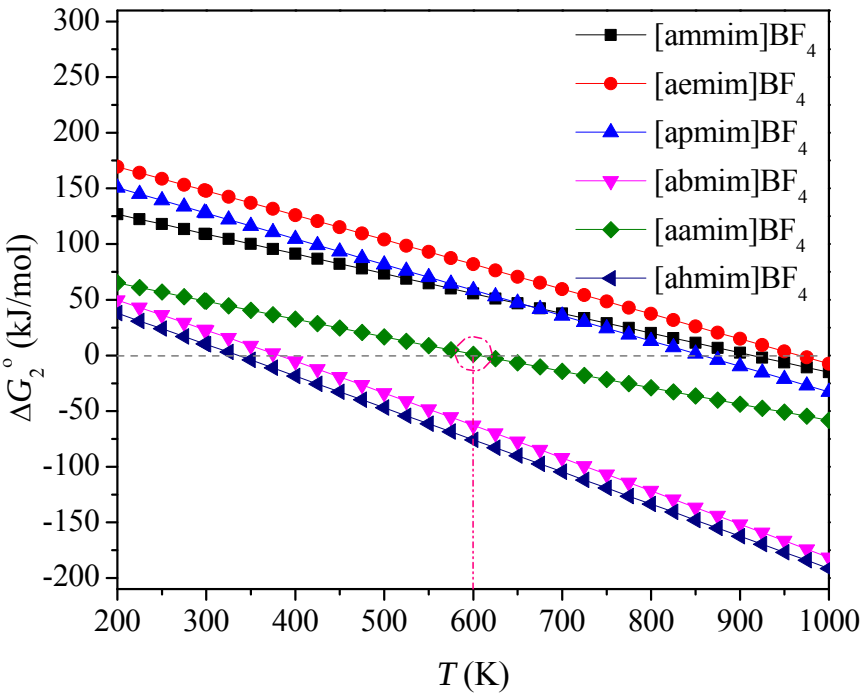

Figure S1. Standard Gibbs free energy of Step 2 (ΔG_2^{Θ}) as a function of temperature in a range of 200-1000 K. The desorption of CO_2 has an increasing priority over Step 2 with the increasing temperature

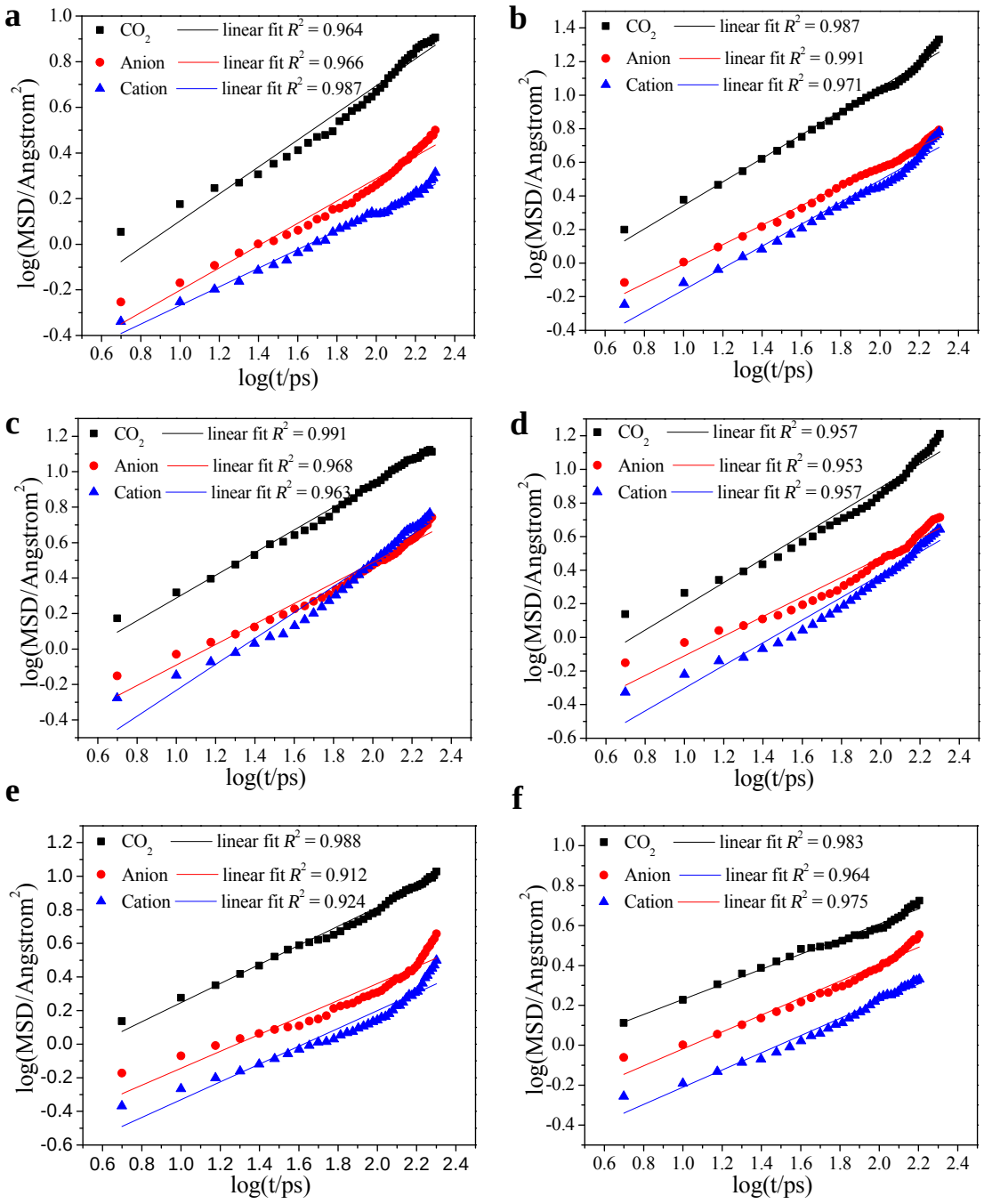

Figure S2. Relationship between log(MSD) and log(t) for the AIIL-CO_2 systems: a. [ammim]BF_4-CO_2, b. [aemim]BF_4-CO_2, c. [apmim]BF_4-CO_2, d. [abmim]BF_4-CO_2, e. [aamim]BF_4-CO_2, and f. [ahmim]BF_4-CO_2

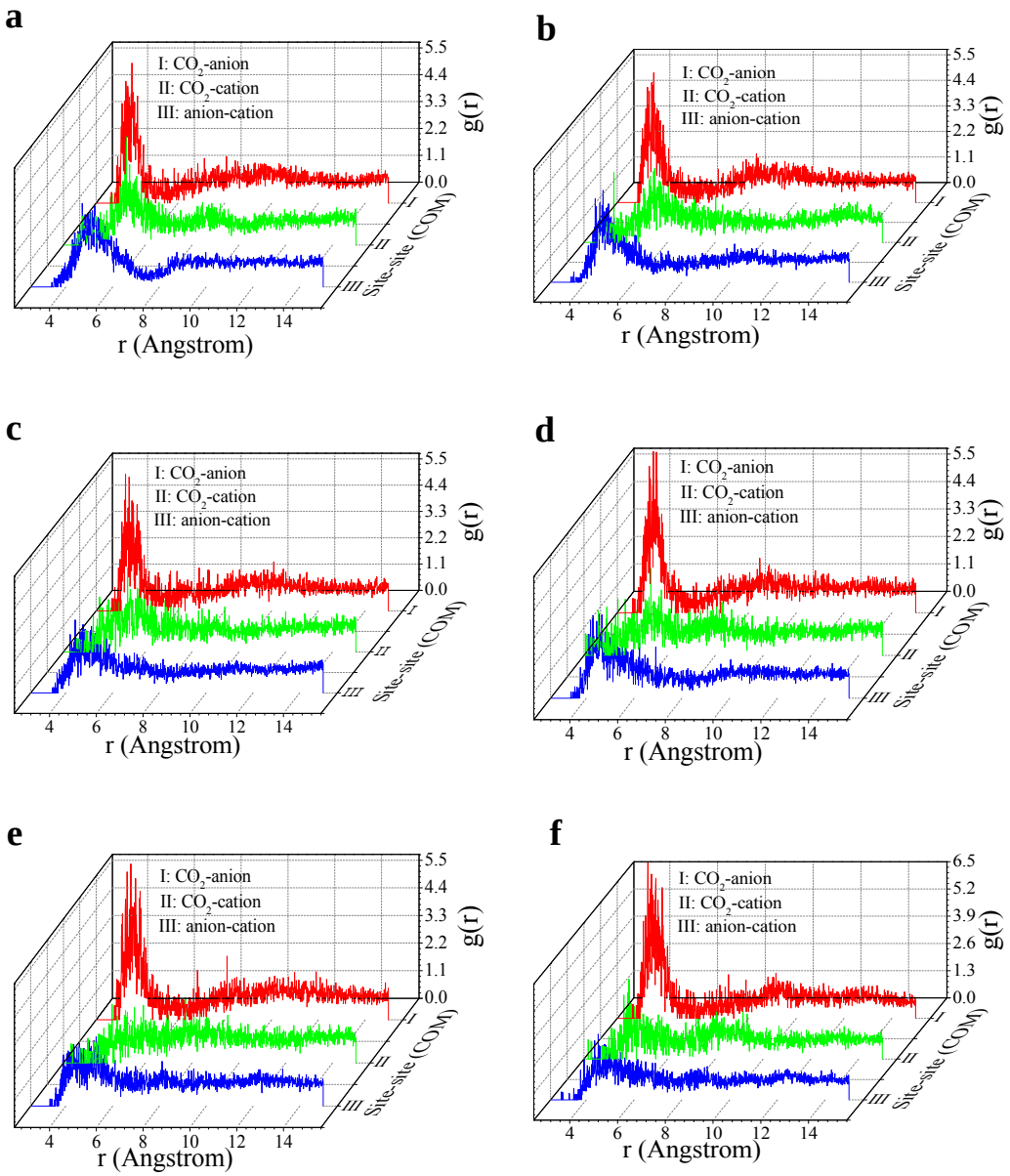

Figure S3. Center-of-mass radial distribution functions (RDFs) of AIIL-CO_2 systems: a. [ammim]BF_4-CO_2, b. [aemim]BF_4-CO_2, c. [apmim]BF_4-CO_2, d. [abmim]BF_4-CO_2, e. [aamim]BF_4-CO_2, and f. [ahmim]BF_4-CO_2