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The electronic supplementary information file

For

Capturing the effect of $[PF_3(C_2F_5)_3]^-$ vs. $[PF_6]^-$, flexible anion vs. rigid, and scaled charge vs. unit on the transport properties of $[bmim]^+$-based ionic liquids: a comparative MD study

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Table S1. Calculated cation and anion diffusion coefficients, D_i (in 10^{-11} m^2 s^{-1}), from the slope of MSD plots (values of β are in the parentheses) and integration of the VACFs (values of errors are in the parentheses) and the calculated ionic conductivity from the Nernst–Einstein, σ_{NE}, and Green–Kubo relations, σ_{GK}, (in mS cm^{-1}) along with the experimental data at 400 K.

ILs	Scaling factor	Volume ($10^{-20}cm^3$)	MSD		VACF		D_{Exp}		σ (mS cm^{-1})			σ_{Exp} (mS cm^{-1})
									σ_{NE}		σ_{GK}	
			D_+ (β)	D_- (β)	D_+	D_-	D_+	D_-	MSD	VACF		
[bmim][PF_6]	Unit	5.38	3.65 (0.88)	3.39 (0.94)	5.26 (± 0.34)	4.66 (± 0.61)	20.92[a]	17.86[a]	9.12	12.69 (± 1.22)	9.74 (± 0.31)	32.5[b]
	0.85	5.58	17.34 (0.99)	16.69 (1.04)	19.23 (± 0.33)	17.61 (± 0.24)			42.54	46.05 (± 0.75)	32.05 (± 4.74)	
	0.8	5.65	26.39 (0.96)	25.46 (1.00)	27.75 (± 1.09)	27.08 (± 0.68)			64.01	67.62 (± 2.21)	47.32	
[bmim][FAP]	Unit	9.63	6.54 (0.96)	5.91 (1.05)	10.62 (± 0.71)	8.32 (± 0.26)			9.02	13.71 (± 0.71)	13.51 (± 0.12)	42.8[c]
	0.8	9.88	27.21 (1.01)	20.69 (1.02)	31.79 (± 3.82)	26.79 (± 4.03)			33.79	41.33 (± 5.21)	40.93 (± 2.04)	

[a] Tokuda et al.[1] [b] Zech et al.[2] at 398.15 K

[c] Nazet et al.[3] for [emim][FAP]) at 398.15 K (for comparison)

Table S2. Calculated cation and anion diffusion coefficients, D_i (in 10^{-11} m^2 s^{-1}) from the slope of MSD plots (values of β are in the parentheses) and integration of the VACFs (values of errors are in the parentheses) together with the cationic transference number, t_+, for [bmim][PF_6] and [bmim][FAP] ILs at 400 K and 1 atm.

IL ([bmim][X])	Charge model	Anion model	MSD plots			Integration of the VACFs		
			D_+ (β)	D_- (β)	t_+	D_+	D_-	t_+
[bmim][PF_6]	Unit	Rigid	2.88 (0.95)	1.82 (0.94)	0.61	4.56 (± 0.46)	2.93 (± 0.35)	0.61
		Flexible	3.65 (0.88)	3.39 (0.94)	0.52	5.26 (± 0.34)	4.66 (± 0.61)	0.53
	Scaled 0.85	Rigid	13.63 (1.01)	10.34 (1.01)	0.57	15.65 (± 0.37)	11.80 (± 0.40)	0.57
		Flexible	17.34 (0.99)	16.69 (1.04)	0.51	19.23 (± 0.33)	17.61 (± 0.24)	0.52
[bmim][FAP]	Unit	Rigid	4.65 (1.05)	3.00 (0.96)	0.61	6.91 (± 0.88)	4.91 (± 0.24)	0.58
		Flexible	6.54 (0.96)	5.91 (1.05)	0.53	10.62 (± 0.71)	8.32 (± 0.26)	0.56
	Scaled 0.80	Rigid	20.08 (1.00)	14.58 (0.98)	0.58	24.16 (± 2.26)	17.41 (± 1.90)	0.58
		Flexible	27.21 (1.01)	20.69 (1.02)	0.57	31.79 (± 2.82)	26.79 (± 2.61)	0.54

Table S3. Computed values of D_+/D_- and HAP derived for pure [bmim][PF_6] and [bmim][FAP] from the simulations with different studied models at 400 K.

IL ([bmim][X])	Charge model	Anion model	MSD		VACF		Other works	
			D_+ / D_-	HAP[a]	D_+ / D_-	HAP[a]	D_+ / D_-	HAP
[bmim][PF_6]	Unit	Rigid	1.58	2.08	1.56	2.06	1.15[b] 1.13[c] 1.27[b]	1.50[b] 1.47[c] 1.65[b]
		Flexible	1.08	1.42	1.13	1.49		
	Scaled 0.85	Rigid	1.32	1.74	1.33	1.75		
		Flexible	1.04	1.37	1.09	1.44		
[bmim][FAP]	Unit	Rigid	1.55	1.38	1.41	1.25		
		Flexible	1.11	0.98	1.28	1.13		
	Scaled 0.80	Rigid	1.38	1.23	1.39	1.24		
		Flexible	1.32	1.17	1.19	1.06		

[a] $r_{[bmim]^+}$ = 0.335 nm, $r_{[PF6]^-}$ = 0.254 nm, $r_{[FAP]^-}$ = 0.377 nm[4-6]

[b] Diffusion coefficients of ions from ref. 7.

[c] Diffusion coefficients of ions from ref. 8.

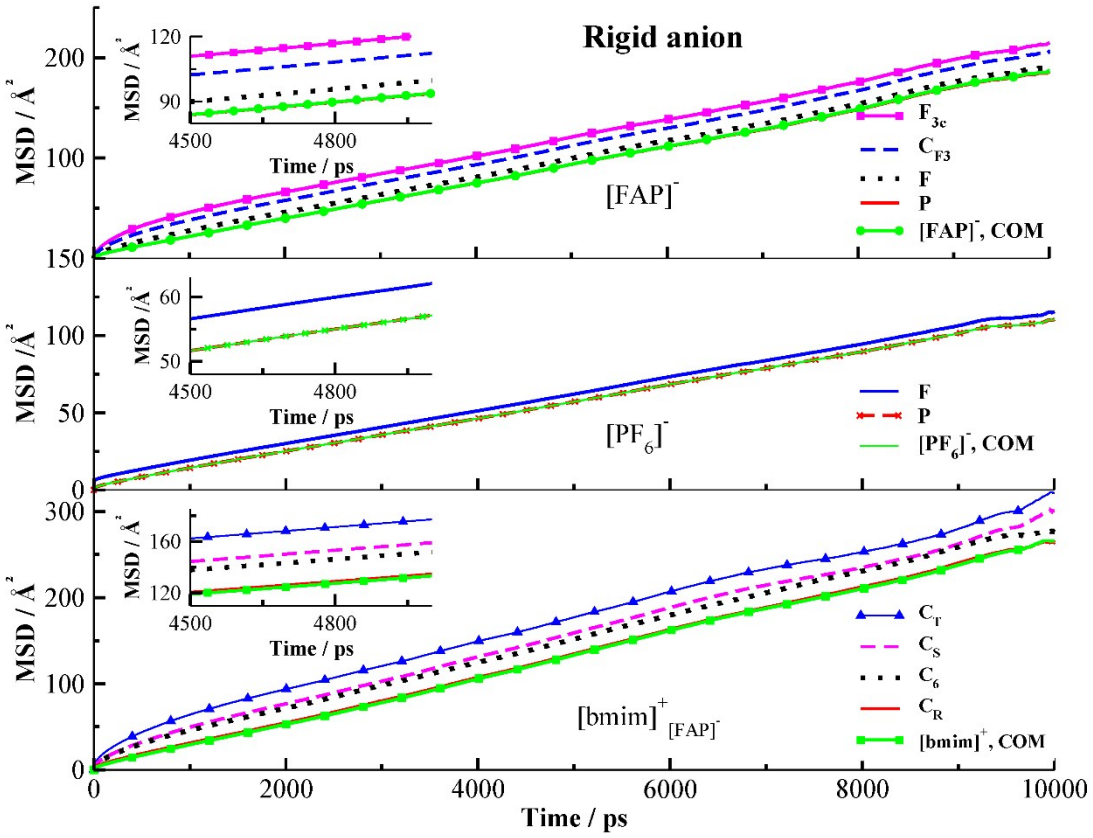

Fig. S1. The MSDs for the COM and some atomic sites of rigid $[PF_6]^-$, rigid $[FAP]^-$ and flexible $[bmim]^+$ at 400 K.

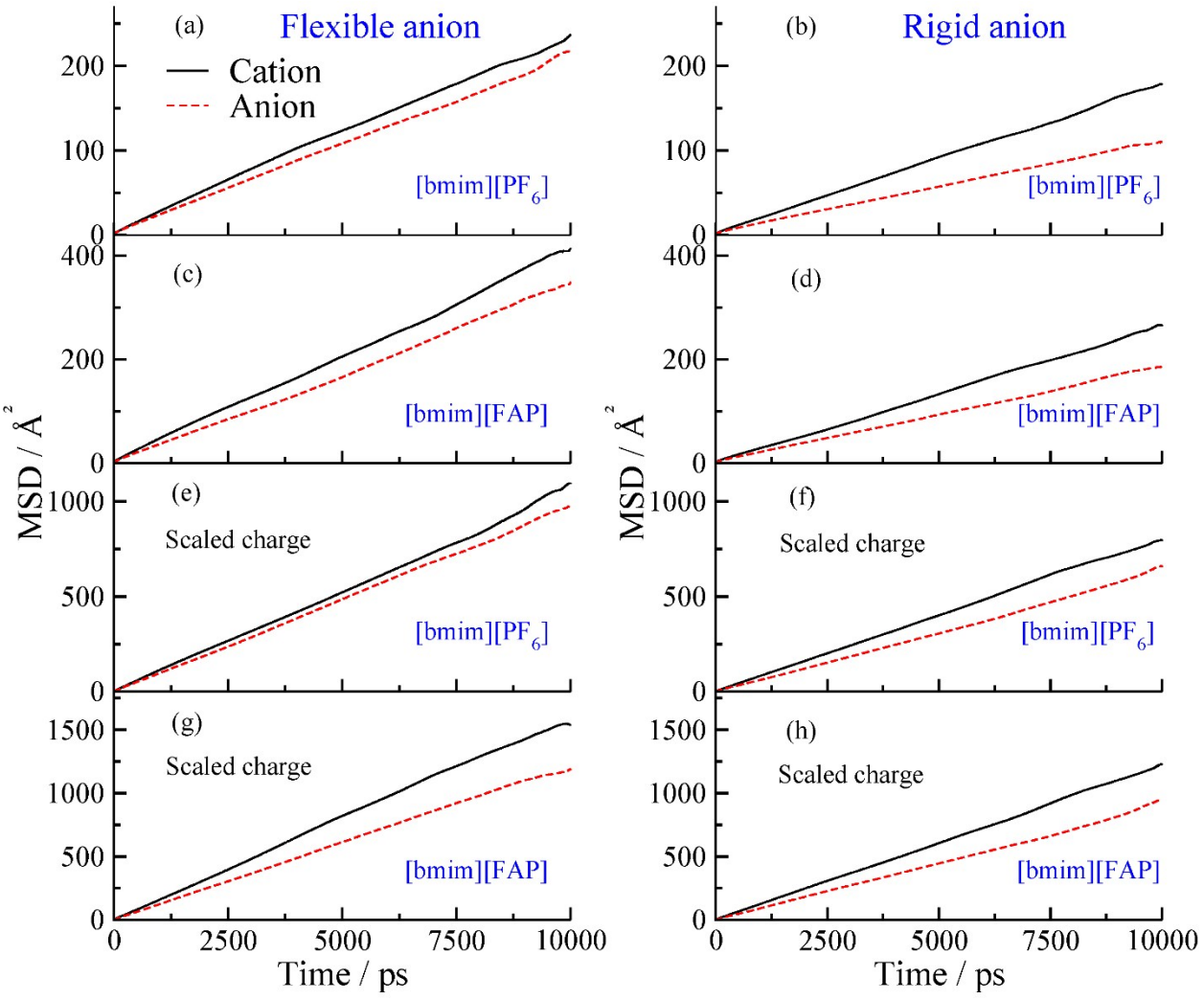

Fig. S2. The calculated COM MSDs of flexible $[bmim]^+$ and both flexible and rigid anions of two ILs at 400 K. The panels (a-d) are related to the unit charge model, and the panels (e-h) are related to the scaled charge model.

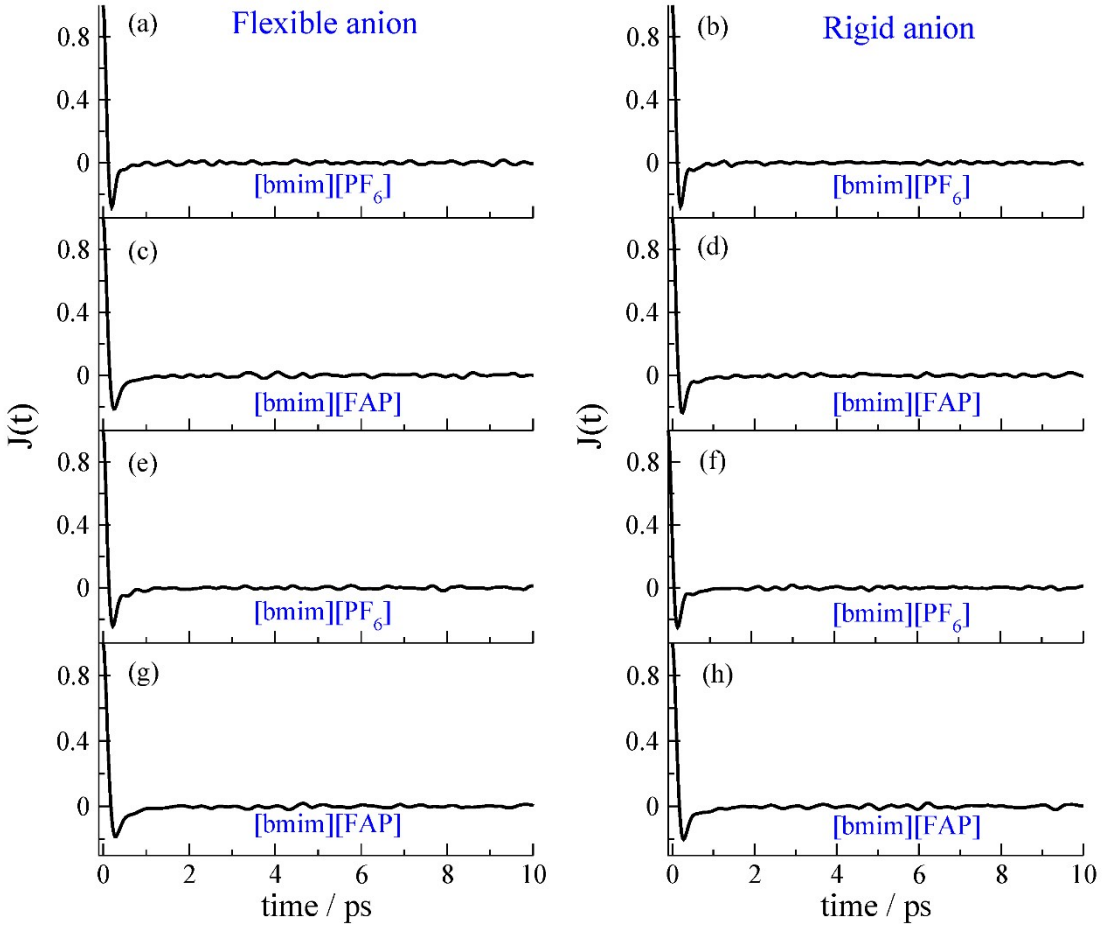

Fig. S3. The calculated normalized electric-current autocorrelation functions. Only the functions are shown up to 10 ps. The panels (a-d) are related to the unit charge model, and the panels (e-h) are related to the charge-scaled model.

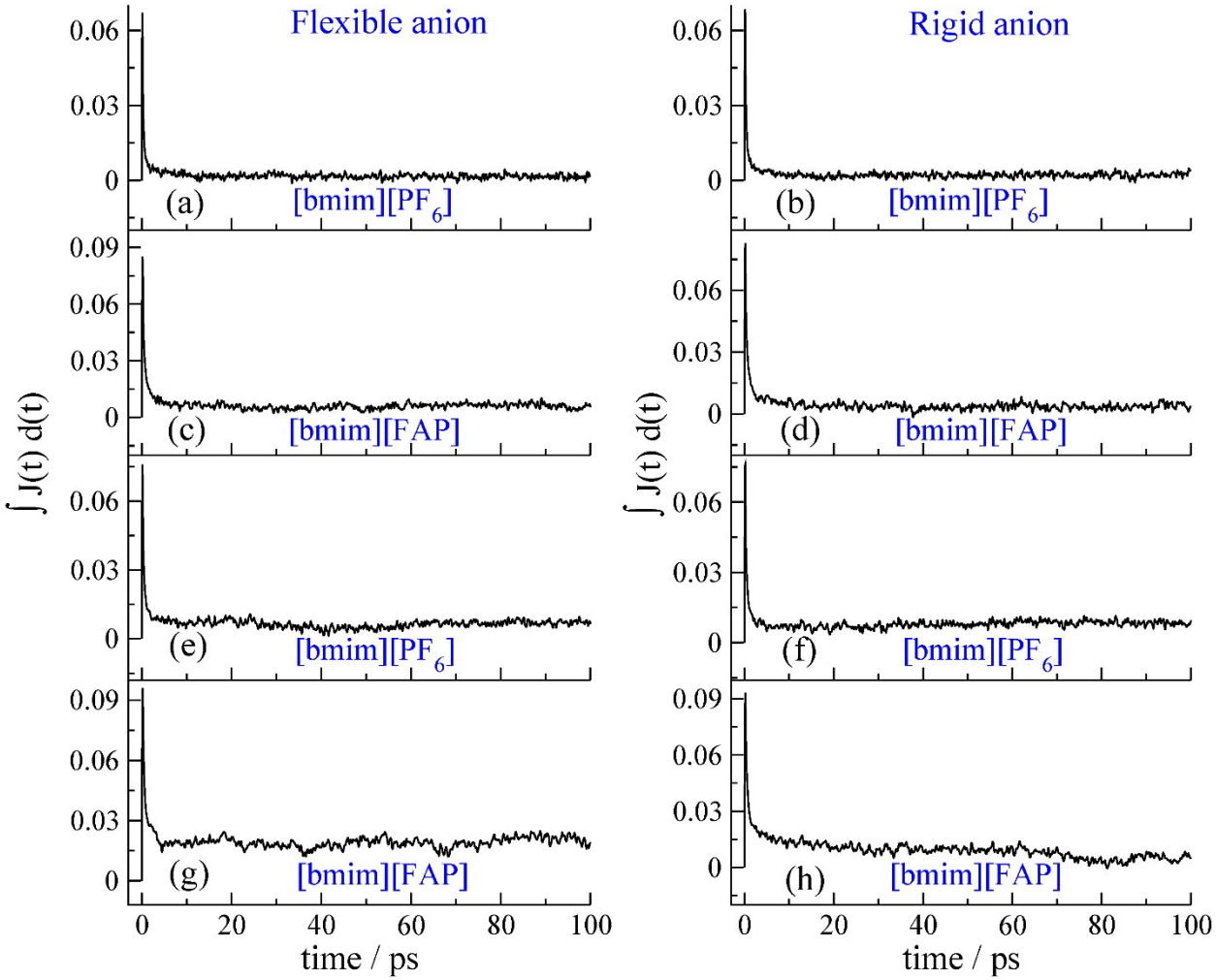

Fig. S4. The calculated integrals of the normalized electric-current autocorrelation functions. The panels (a-d) are related to the unit charge model, and the panels (e-h) are related to the charge-scaled model.

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