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外电场作用下离子液体振动光谱变化的分子动力学模拟研究

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Atomistic Insight into the Vibrational Spectrum Change of Ionic Liquids under External Electric Field

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Table S1 The assignments for vibrational spectra of $[Emim]^+$ cation, $[PF_6]^-$ anion and $[Emim][PF_6]$ IL with 0 $V \cdot nm^{-1}$ EEF.

Wavenumber (cm^{-1}) [a]	Assignment [b]
50 vvs	Cat-An bend
83 vs	Cat-An stretch
183 w	tors Et
266 vw	γ N-Me
416 w br	δ PF_6
433 vvs	r N-Et, r N-Me
583 vw	ν PF_6
632 s	γ N-Et, γ N-Me
783 vs	r CH_2, r CH_3 (Et), γ C4-H, γ C5-H
	ν PF_6
949 vs	ν CC (Et), γ C2-H
	ν PF_6
1132 m	r CH_3 (Me), r CH_2, CH_3 (Et)
1298 vw	r C2-H, C4-H, C5-H, t CH_2
1465 m	δ CH_3 (Me)
1665 m	ν C=C, ν_{as} NC2N
3196 m	ν CH_3 (Me)
3396 m	ν C2-H2
	ν C4-H4, C5-H5

[a] Labels: m, medium; s, strong; w, weak; v, very; sh, shoulder; br, broad. [b] Labels: ν, stretch; δ, bend; γ, out of plane; r, rocking; t, twisting; tors, torsion; Et, ethyl; Me, methyl; as, anti-symmetrical.

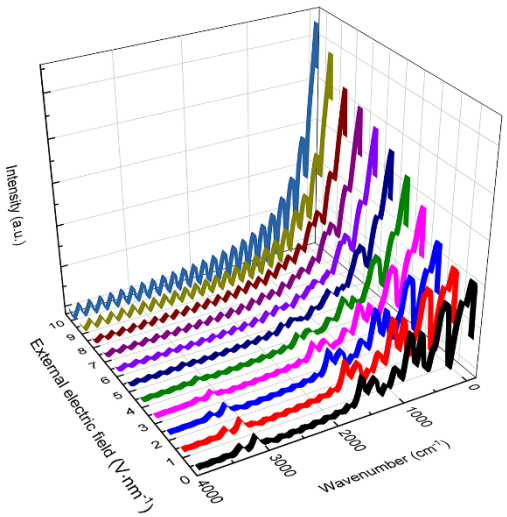

Fig. S1 Vibrational spectra (arbitrary units) in the range of 10 to 4000 cm^{-1} for $[Emim][PF_6]$ IL with a series of different EEFs varying from 0 to 10 $V \cdot nm^{-1}$ with interval of 1 $V \cdot nm^{-1}$, which are displayed by a three-dimensional ribbon graph.

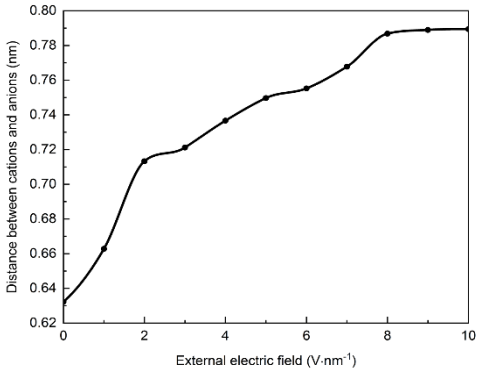

Fig. S2 Average distances between anions and cations of [Emim][PF_6] IL in the simulation system under varied EEFs ranging from 0 to 10 V·nm^{-1}.

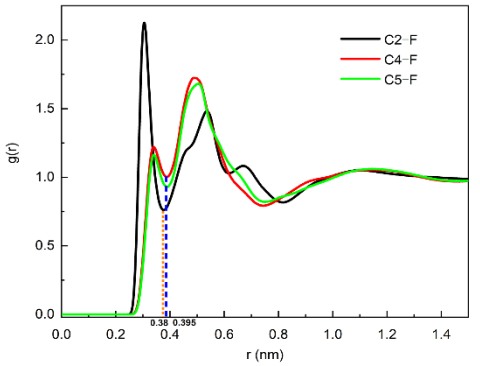

Fig. S3 RDFs between carbon atoms in cationic imidazole ring ($[Emim]^+$) and fluorine atom on $[PF_6]^-$ anion for the bulk [Emim][PF_6] IL at 350 K and 0 V·nm^{-1} EEF.