Electronic supplementary information for

Systematic analysis of various ionic liquids by attenuated total reflectance spectroscopy (145–450 nm) and quantum chemical calculations

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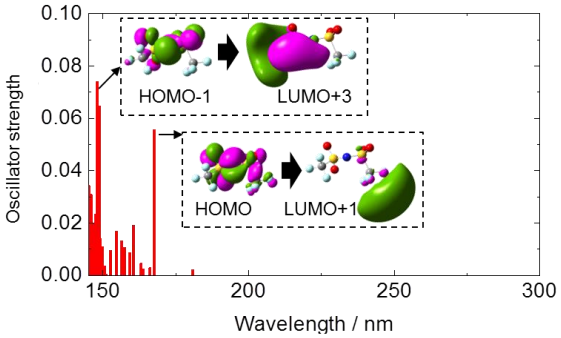

Fig. S1 Calculated vertical transitions of $[TFSA]^-$ and the most relevant molecular orbitals.

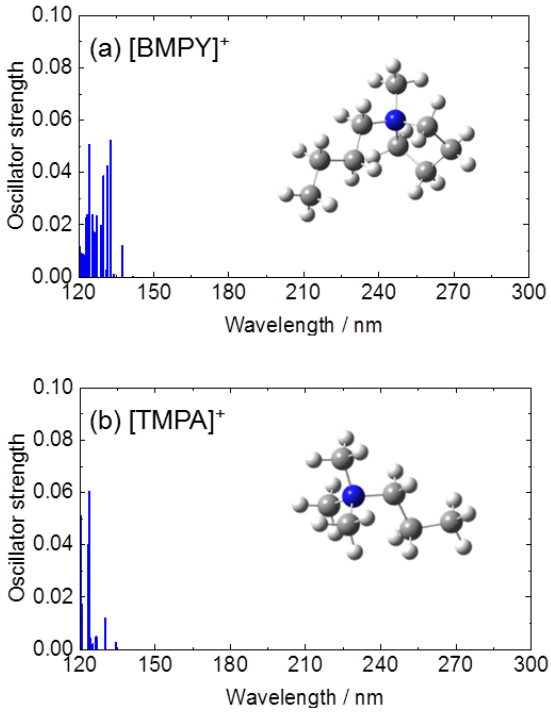

Fig. S2 Calculated vertical transitions of (a) $[BMPY]^+$ and (b) $[TMPA]^+$.

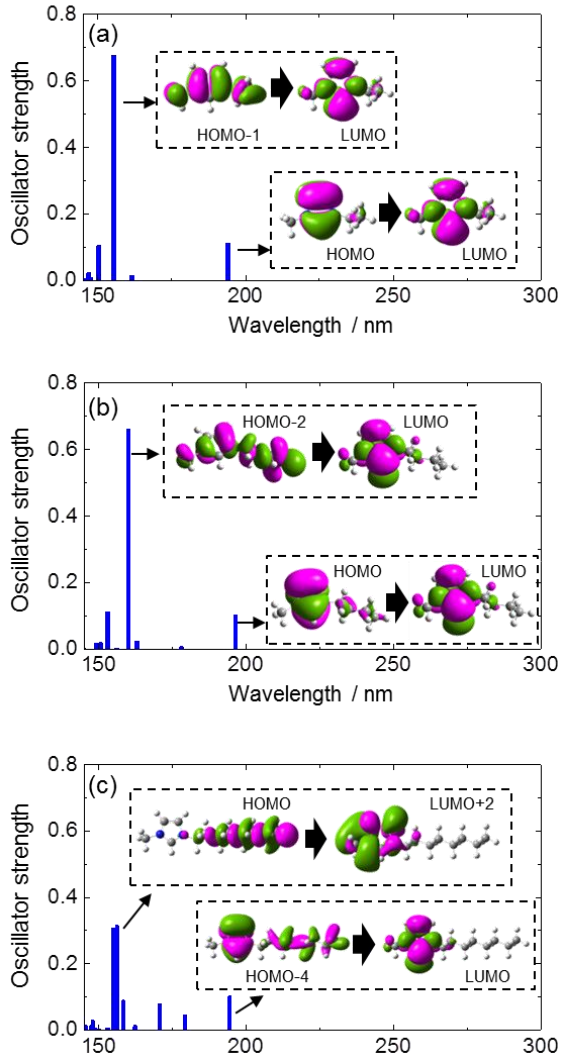

Fig. S3 Calculated vertical transitions of (a) $[EMIM]^+$, (b) $[BMIM]^+$, and (c) $[OMIM]^+$ and the most relevant molecular orbitals.

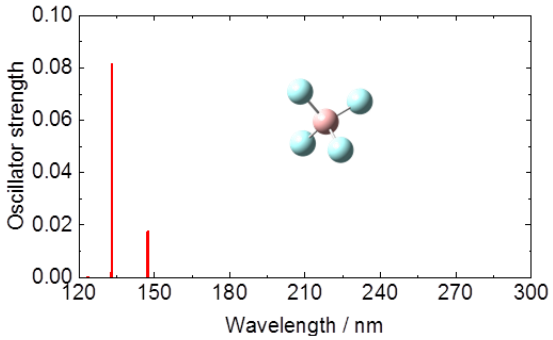

Fig. S4 Calculated vertical transitions of $[BF_4]^-$.

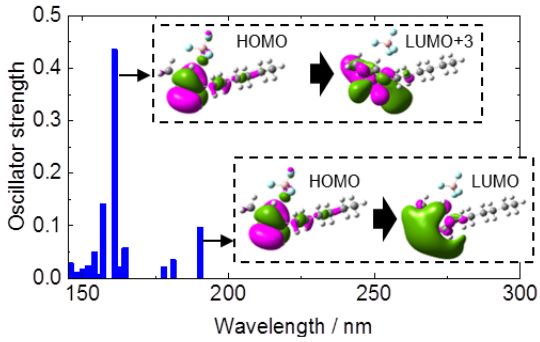

Fig. S5 Calculated vertical transitions of [BMIM][BF_4] and the most relevant molecular orbitals.

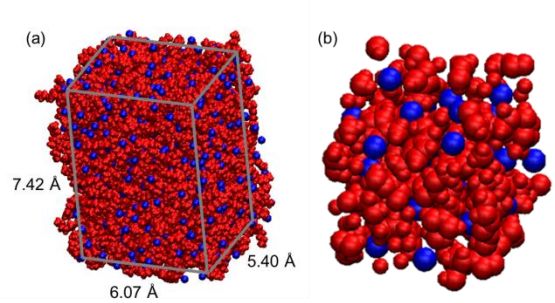

Fig. S6 (a) Snapshot of a simulation box containing 800 ion pairs of [BMIM]I and (b) a representative enlarged view. Red balls represent atoms composing BMIM, and blue balls represent iodide. After a 5.8-ns equilibration run, a 5-ns production run was carried out using the GROMACS-5.0.7 package.[1] Force field parameters were taken from the CLaP force field.[2,3] All C–H bonds were constrained using the LINCS algorithm.[4] The particle-mesh Ewald method[5] was used to treat long-range electrostatic interactions. A cut-off distance of 1.2 nm was used for non-bonded forces, and eriodic boundary conditions were employed. Newton's equation of motion was integrated using the leapfrog algorithm with a time step of 1 fs, and the obtained configuration was saved after every 3000 time steps. Simulations were performed in the NPT ensemble using the Nose-Hoover thermostat[6,7] to maintain a temperature of 300 K, and the Parrinello-Rahman barostat[8] was used to maintain a pressure of 1 bar.

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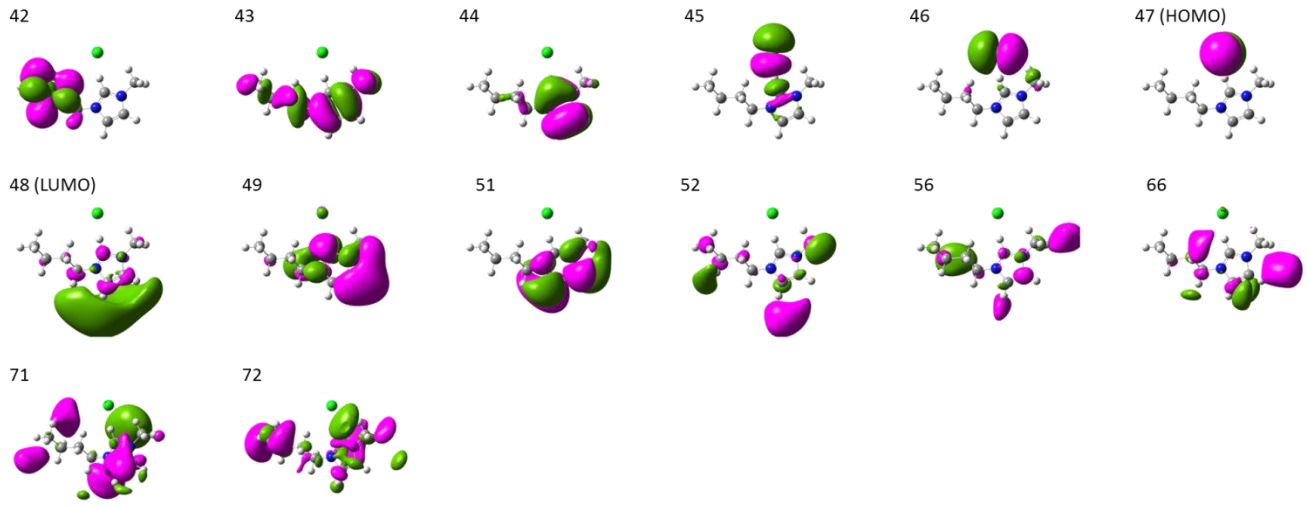
Table S1. Twenty main transition energies, oscillator strengths, main initial states, and main final states calculated for (a) [OMIM]Cl, (b) [HMIM]Br, and (c) [BMIM]I. Gray bands represent CT transitions.

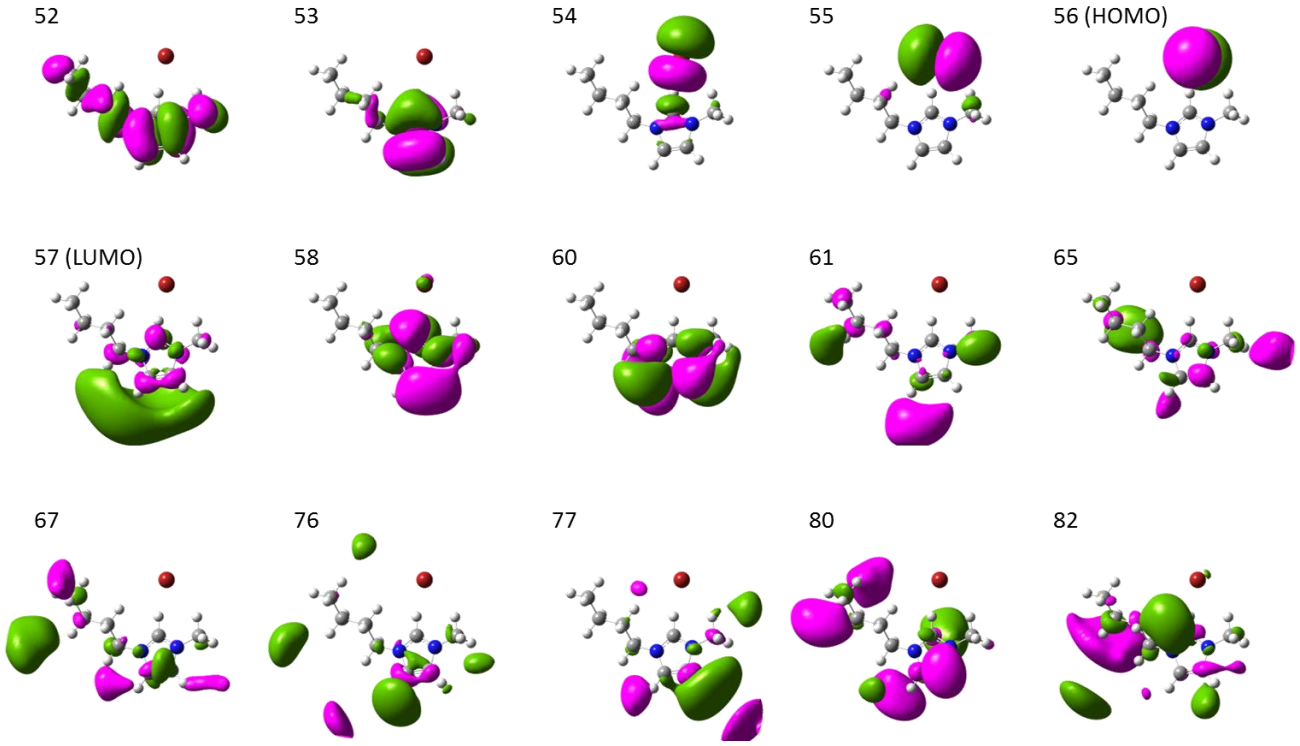
(a) [OMIM]Cl

Wavelength/nm	Energy/eV	Oscillator strength	Main initial states	Main final states
271.67	4.56	0.0285	47	49
237.07	5.23	0.0196	47	48
215.16	5.76	0.0200	47	52
191.69	6.47	0.0744	45	56
188.89	6.56	0.0809	44	49
181.83	6.82	0.0304	44	48
181.71	6.82	0.0250	44	48
181.23	6.84	0.0374	44	51
160.26	7.74	0.0454	43	51
160.02	7.75	0.0697	43	51
158.80	7.81	0.2176	43	49
158.27	7.83	0.0674	46	71
157.70	7.86	0.0423	45	66
157.10	7.89	0.0293	47	72
155.34	7.98	0.0800	46	72
153.99	8.05	0.0294	43	48
153.49	8.08	0.0382	47	71
153.10	8.10	0.0503	43	48
152.71	8.12	0.0356	44	52
147.48	8.41	0.0252	42	48



(b) [HMIM]Br

Wavelength/nm	Energy/eV	Oscillator strength	Main initial states	Main final states
300.36	4.13	0.0288	56	58
231.34	5.36	0.0283	56	61
228.32	5.43	0.0283	55	61
206.24	6.01	0.0327	55	65
203.18	6.10	0.0533	54	65
190.68	6.50	0.0537	55	67
190.07	6.52	0.0856	53	58
180.84	6.86	0.0504	53	60
180.12	6.88	0.0294	53	57
159.32	7.78	0.1193	52	60
159.26	7.79	0.0409	54	80
159.12	7.79	0.0330	54	76
158.94	7.80	0.0513	54	80
158.24	7.84	0.2779	52	58
157.96	7.85	0.0734	56	77
155.99	7.95	0.0267	55	82
154.54	8.02	0.0332	56	80
152.80	8.11	0.0399	52	57
151.87	8.16	0.0424	52	60
147.96	8.38	0.0313	54	82



(c) [BMIM]I

Wavelength/nm	Energy/eV	Oscillator strength	Main initial states	Main final states
331.04	3.75	0.0431	65	66
324.39	3.82	0.0762	63	66
267.16	4.64	0.0402	63	66
190.20	6.52	0.0634	62	66
181.28	6.84	0.0508	64	83
176.31	7.03	0.0540	63	86
173.03	7.17	0.0380	65	85
164.25	7.55	0.0454	62	68
163.36	7.60	0.0436	64	95
162.45	7.63	0.0419	65	88
161.84	7.66	0.0541	62	69
160.22	7.74	0.0392	62	68
159.13	7.79	0.0521	65	94
158.44	7.83	0.0873	65	97
158.19	7.84	0.0634	65	94
157.81	7.86	0.0406	64	97
157.43	7.88	0.0459	64	94
154.37	8.03	0.0796	61	68
151.61	8.18	0.0905	61	67
147.18	8.42	0.0880	62	72