Supporting Information for

Interionic Interactions of Binary Gels Consisting of Pyrrolidinium-Based Zwitterionic Compounds and Lithium Salts

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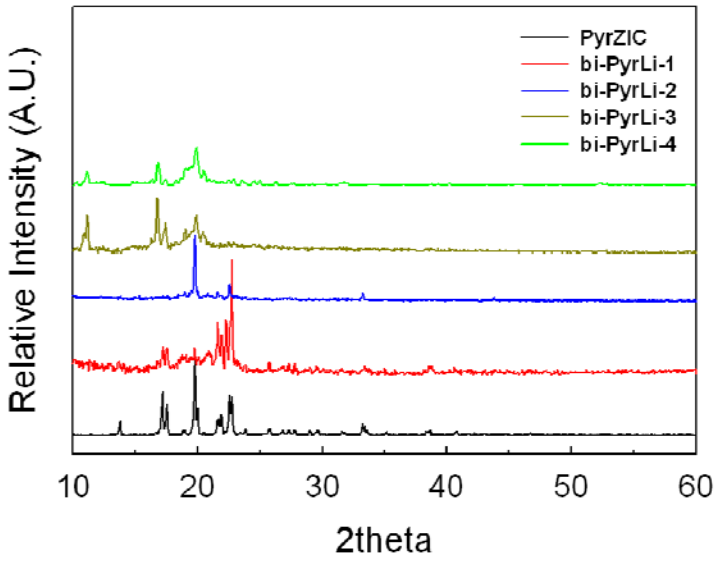

Figure S1. XRD patterns of PyrZIC and bi-PyrLis.

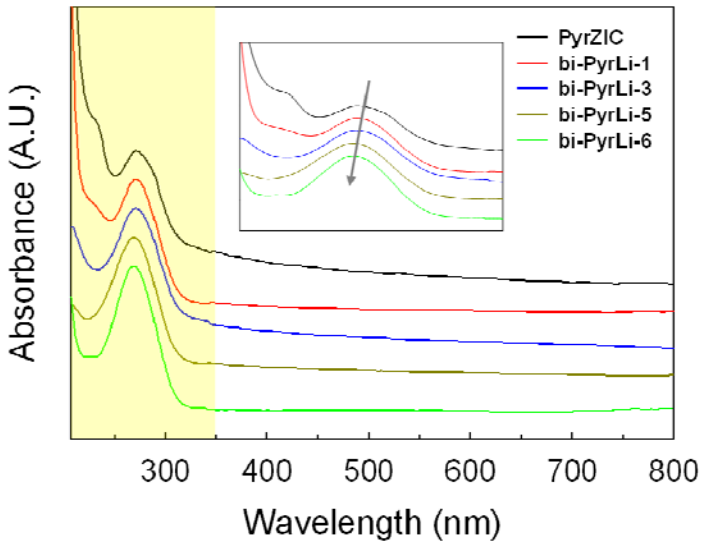

Figure S2. UV-vis spectra of PyrZIC and bi-PyrLis. Inset is the enlarged image of yellow box.

Table S1. Bond distances, bond angles, and dihedral angles of PyrZIC-LiTFSI at the respectively optimized state. Atom numbering of PyrZIC-LiTFSI at the respectively optimized state below. Symbol indicates atom, NA, NB, and NC indicates nearest atoms, bond indicates the distance between selected atom and NA, angle indicates the angle of NA-(selected atom)-NB, and dihedral indicates the dihedral angle of (selected atom)-(the plane composed of NA, NB, and NC). Light and dark gray, blue, red, yellow, cyan, and pink colors represent hydrogen, carbon, nitrogen, oxygen, sulfur, fluoride, and lithium atoms, respectively.

#	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	C						
2	C	1			1.528826		
3	N	2	1		1.530197	104.966549	
4	C	3	2	1	1.525797	102.423165	−39.178932
5	C	4	3	2	1.535859	105.886795	35.985329
6	H	1	2	3	1.088926	109.615840	147.537622
7	H	2	1	5	1.089016	112.633277	−87.404154
8	H	4	3	2	1.088396	106.629768	−83.431807
9	C	3	2	1	1.520351	112.572316	−157.123710
10	C	9	3	2	1.539896	114.750985	−67.585927
11	H	9	3	2	1.087419	105.258705	54.443616
12	H	9	3	2	1.091732	105.785559	169.112299
13	C	10	9	3	1.532928	113.196566	136.036189
14	H	10	9	3	1.093481	109.804860	−101.933871
15	H	10	9	3	1.092173	111.353054	16.186378
16	H	13	10	9	1.091502	113.471948	45.225936
17	H	13	10	9	1.090643	110.315725	167.362293
18	S	13	10	9	1.831018	112.044658	−76.356504
19	O	18	13	10	1.467920	106.842625	−172.130308
20	O	18	13	10	1.477016	104.956898	−46.499362
21	O	18	13	10	1.526669	103.171316	69.830061
22	H	5	4	3	1.091360	111.618935	101.807213
23	H	1	2	3	1.092041	111.369822	−93.246982
24	H	5	4	3	1.089427	109.310378	−139.230947
25	H	4	3	2	1.090017	108.411990	159.821939
26	H	2	1	5	1.087820	115.658319	148.419205
27	C	3	2	1	1.497311	110.880695	77.853527
28	H	27	3	2	1.089695	108.766482	−177.978223
29	H	27	3	2	1.087753	109.331820	−58.211575
30	H	27	3	2	1.087276	109.526023	61.837427
31	Li	21	18	13	1.810464	137.453212	136.568199
32	F	31	21	18	5.538157	111.015135	−157.787899
33	C	31	21	18	4.518194	116.848080	−149.144971
34	F	33	31	21	1.332733	103.095678	79.908316
35	F	33	31	21	1.331820	87.894734	−170.778398
36	S	33	31	21	1.889832	27.636189	−25.567041
37	O	36	33	31	1.460615	104.617867	144.337125
38	O	36	33	31	1.477481	104.586220	19.940227
39	N	36	33	31	1.609717	103.912345	−101.373070
40	S	39	36	33	1.611890	126.265275	114.591716
41	O	40	39	36	1.477150	114.354302	13.855005
42	O	40	39	36	1.454721	108.367640	148.184824
43	C	40	39	36	1.891017	105.730592	−99.815465
44	F	43	40	39	1.332175	110.031935	−51.851330
45	F	43	40	39	1.331851	108.966297	−171.715785
46	F	43	40	39	1.333440	110.023728	68.558635

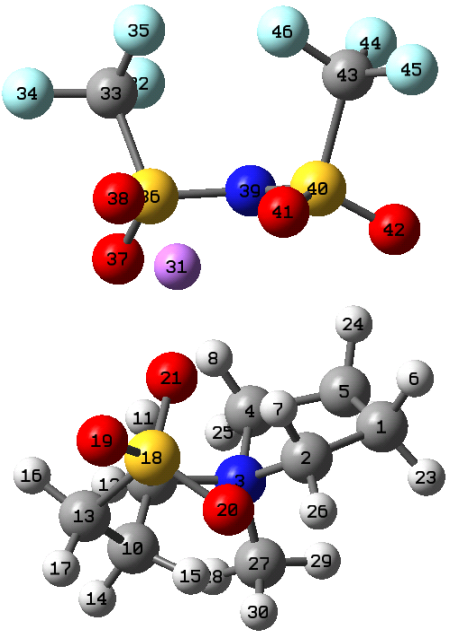

Table S2. Bond distances, bond angles, and dihedral angles of LiTFSI -LiTFSI at the respectively optimized state. Atom numbering of LiTFSI-LiTFSI at the respectively optimized state below. Symbol indicates atom, NA, NB, and NC indicates nearest atoms, bond indicates the distance between selected atom and NA, angle indicates the angle of NA-(selected atom)-NB, and dihedral indicates the dihedral angle of (selected atom)-(the plane composed of NA, NB, and NC). Gray, blue, red, yellow, cyan, and pink colors represent carbon, nitrogen, oxygen, sulfur, fluoride, and lithium atoms, respectively.

#	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	C						
2	F	1			1.329870		
3	F	1	2		1.327838	109.708683	
4	F	1	3	2	1.336781	109.351620	-119.781405
5	S	1	3	2	1.891906	110.140773	119.822746
6	O	5	1	3	1.443514	106.187815	-61.422807
7	O	5	1	6	1.482393	103.639783	-125.784131
8	N	5	1	7	1.617829	103.910014	-118.261986
9	S	8	5	1	1.581466	126.574119	98.617240
10	O	9	8	5	1.482905	116.724228	-7.199285
11	O	9	8	5	1.476554	111.084135	126.772582
12	C	9	8	5	1.889997	103.925352	-122.752150
13	F	12	9	8	1.325920	109.794025	-57.018675
14	F	12	9	8	1.329360	108.458805	-177.050927
15	F	12	9	8	1.329808	109.329131	63.445565
16	Li	7	5	1	1.882344	133.609606	-103.810198
17	O	16	7	5	1.888321	128.949844	-113.569899
18	S	17	16	7	1.476557	128.656404	81.164063
19	C	18	17	16	1.890011	103.308273	-137.874959
20	O	18	17	16	1.482901	114.635883	-23.741444
21	N	18	17	16	1.581472	111.085049	111.252049
22	F	19	18	17	1.329354	108.457377	60.977780
23	F	19	18	17	1.325913	109.794252	-59.053490
24	F	19	18	17	1.329810	109.329532	-179.519335
25	Li	11	9	8	1.888260	128.657422	-111.172053
26	S	21	18	17	1.617838	126.567565	-126.793718
27	O	26	21	18	1.482390	112.949428	13.113459
28	O	26	21	18	1.443509	109.929879	148.185197
29	C	26	21	18	1.891911	103.917523	-98.527334
30	F	29	26	21	1.327842	110.140562	-54.512835
31	F	29	26	21	1.329860	108.873140	-174.842786
32	F	29	26	21	1.336796	109.516442	65.781864