

Table S1. CM5 partial charges and spin density values of isolated electrolyte molecules (orders coincide with atom numbers in Figure 2)

Molecule		Partial Charge (e)		Spin Density
		Initial State	Oxidized State	Oxidized State
DME_ttt	1	-0.14	-0.10	0.02
	2	0.11	0.14	0.02
	3	0.10	0.14	0.01
	4	0.10	0.14	0.00
	5	-0.31	-0.18	0.25
	6	-0.06	0.03	0.17
	7	0.10	0.16	0.02
	8	0.10	0.16	0.02
	9	-0.06	0.03	0.17
	10	0.10	0.16	0.02
	11	0.10	0.17	0.02
	12	-0.31	-0.18	0.25
	13	-0.14	-0.10	0.01
	14	0.10	0.14	0.01
	15	0.11	0.14	0.02
	16	0.10	0.14	0.00
DME_tgt	1	-0.06	0.02	0.16
	2	0.10	0.17	0.03
	3	0.10	0.147	0.02

	4	-0.06	0.02	0.16
	5	0.10	0.17	0.02
	6	0.10	0.16	0.02
	7	-0.31	-0.17	0.26
	8	-0.31	-0.18	0.24
	9	-0.14	-0.10	0.02
	10	0.10	0.14	0.01
	11	0.11	0.14	0.00
	12	0.10	0.13	0.02
	13	-0.14	-0.10	0.01
	14	0.10	0.13	0.01
	15	0.11	0.14	0.00
	16	0.10	0.14	0.01
DOL	1	-0.06	-0.01	0.02
	2	-0.06	-0.01	0.02
	3	0.04	0.16	0.14
	4	0.11	0.16	0.01
	5	0.12	0.17	0.01
	6	0.11	0.17	0.01
	7	0.11	0.16	0.01
	8	0.13	0.25	0.14
	9	0.11	0.25	0.14
	10	-0.30	-0.15	0.26

	11	-0.31	-0.15	0.26
FSI-	1	-0.19	0.03	0.67
	2	0.54	0.64	0.03
	3	0.55	0.64	0.03
	4	-0.40	-0.30	0.07
	5	-0.40	-0.30	0.07
	6	-0.40	-0.30	0.07
	7	-0.40	-0.30	0.07
	8	-0.15	-0.05	0.00
	9	-0.15	-0.06	0.00
TFSI-	1	-0.20	0.00	0.66
	2	0.46	0.53	0.03
	3	0.46	0.54	0.02
	4	-0.40	-0.31	0.09
	5	-0.41	-0.32	0.06
	6	-0.40	-0.32	0.08
	7	-0.41	-0.32	0.06
	8	0.17	0.19	0.00
	9	0.17	0.20	0.00
	10	-0.07	-0.03	0.00
	11	-0.07	-0.03	0.00
	12	-0.07	-0.03	0.00
	13	-0.07	-0.03	0.00

	14	-0.07	-0.03	0.00
	15	-0.07	-0.03	0.00
EDOT	1	-0.17	-0.05	0.24
	2	0.06	0.18	0.21
	3	0.06	0.11	0.03
	4	-0.17	-0.10	0.04
	5	0.05	0.28	0.23
	6	0.13	0.18	0.01
	7	0.13	0.17	0.00
	8	-0.25	-0.21	0.01
	9	-0.25	-0.13	0.20
	10	-0.05	-0.03	0.00
	11	0.12	0.14	0.00
	12	0.13	0.16	0.00
	13	-0.05	-0.02	0.01
	14	0.13	0.16	0.00
	15	0.12	0.15	0.01
FEC	1	0.10	0.15	0.01
	2	-0.04	0.02	0.01
	3	0.14	0.18	0.00
	4	0.14	0.18	0.00
	5	-0.21	-0.12	0.02
	6	-0.21	-0.13	0.02

	7	0.39	0.49	0.05
	8	-0.36	0.07	0.88
	9	-0.12	-0.05	0.00
	10	0.16	0.20	0.00
I ⁻	1	-1.00	0.00	1.00
Pyrrole	1	-0.46	-0.39	0.01
	2	-0.02	0.18	0.37
	3	-0.02	0.18	0.37
	4	0.37	0.41	0.00
	5	-0.17	-0.04	0.10
	6	0.13	0.19	0.02
	7	-0.17	-0.04	0.10
	8	0.13	0.19	0.02
	9	0.11	0.16	0.00
	10	0.11	0.16	0.00
BOB ⁻	1	0.31	0.42	0.15
	2	0.31	0.42	0.15
	3	0.31	0.33	0.00
	4	0.31	0.33	0.00
	5	0.30	0.34	0.01
	6	-0.28	-0.27	0.00
	7	-0.28	-0.27	0.00
	8	-0.28	-0.17	0.09

	9	-0.28	-0.17	0.09
	10	-0.36	-0.17	0.25
	11	-0.36	-0.17	0.25
	12	-0.36	-0.31	0.00
	13	-0.36	-0.31	0.00
DFOB	1	0.30	0.41	0.15
	2	0.30	0.41	0.15
	3	-0.37	-0.19	0.25
	4	-0.37	-0.19	0.25
	5	-0.24	-0.14	0.09
	6	-0.24	-0.14	0.09
	7	-0.21	-0.15	0.00
	8	-0.21	-0.15	0.00
	9	0.05	0.12	0.01

Table S2. CM5 partial charges and spin density values of electrolyte complexes with Li⁺ (orders coincide with atom numbers in Figure 3)

Complex		Partial Charge (e)		Spin Density
		Initial State	Oxidized State	Oxidized State
DME_ttt/Li ⁺	1	-0.11	-0.08	0.01
	2	0.14	0.15	0.01
	3	0.12	0.16	0.00
	4	0.12	0.15	0.00
	5	-0.38	-0.26	0.15
	6	-0.04	0.04	0.19
	7	0.12	0.17	0.02
	8	0.13	0.18	0.01
	9	-0.05	0.03	0.14
	10	0.12	0.18	0.02
	11	0.12	0.17	0.03
	12	-0.30	-0.12	0.34
	13	-0.13	-0.08	0.03
	14	0.10	0.16	0.02
	15	0.12	0.15	0.00
	16	0.10	0.16	0.02
	17	0.82	0.86	0.00
DME_tgt/Li ⁺	1	-0.04	0.03	0.13
	2	0.13	0.19	0.03

	3	0.13	0.17	0.02
	4	-0.04	0.04	0.18
	5	0.13	0.18	0.03
	6	0.13	0.18	0.01
	7	-0.36	-0.27	0.14
	8	-0.36	-0.12	0.36
	9	-0.11	-0.09	0.01
	10	0.12	0.14	0.01
	11	0.13	0.16	0.00
	12	0.12	0.15	0.00
	13	-0.11	-0.08	0.03
	14	0.12	0.15	0.01
	15	0.13	0.16	0.01
	16	0.12	0.15	0.03
	17	0.77	0.85	0.00
DOL/Li ⁺	1	-0.04	0.00	0.01
	2	-0.04	0.02	0.06
	3	0.07	0.16	0.11
	4	0.13	0.16	0.00
	5	0.13	0.18	0.00
	6	0.12	0.20	0.03
	7	0.14	0.20	0.05
	8	0.15	0.24	0.07

	9	0.13	0.25	0.11
	10	-0.37	-0.26	0.05
	11	-0.28	-0.02	0.51
	12	0.86	0.87	0.00
LiFSI	1	-0.15	0.04	0.67
	2	0.59	0.65	0.03
	3	0.59	0.68	0.03
	4	-0.44	-0.35	0.05
	5	-0.36	-0.27	0.07
	6	-0.36	-0.28	0.07
	7	-0.43	-0.29	0.08
	8	-0.11	-0.04	0.00
	9	-0.11	-0.04	0.00
	10	0.77	0.88	0.00
LiTFSI	1	-0.17	0.03	0.72
	2	0.50	0.58	0.04
	3	0.50	0.56	0.03
	4	-0.45	-0.35	0.07
	5	-0.37	-0.29	0.05
	6	-0.45	-0.35	0.07
	7	-0.37	-0.29	0.02
	8	0.18	0.22	0.00
	9	0.18	0.21	0.00

	10	-0.05	-0.01	0.00
	11	-0.05	-0.01	0.00
	12	-0.05	-0.01	0.00
	13	-0.05	-0.02	0.00
	14	-0.05	-0.01	0.00
	15	-0.05	-0.01	0.00
	16	0.75	0.76	0.00
EDOT/Li ⁺	1	-0.15	-0.02	0.27
	2	0.07	0.19	0.20
	3	0.07	0.11	0.01
	4	-0.15	-0.06	0.09
	5	0.10	0.30	0.19
	6	0.14	0.19	0.01
	7	0.15	0.19	0.01
	8	-0.31	-0.27	0.00
	9	-0.24	-0.13	0.20
	10	-0.03	-0.01	0.00
	11	0.14	0.16	0.00
	12	0.15	0.17	0.00
	13	-0.04	-0.01	0.01
	14	0.14	0.17	0.00
	15	0.13	0.16	0.01
	16	0.84	0.86	0.00

FEC/Li ⁺	1	0.12	0.16	0.01
	2	-0.02	0.11	0.24
	3	0.16	0.29	0.13
	4	0.16	0.30	0.15
	5	-0.18	-0.02	0.40
	6	-0.18	-0.12	0.00
	7	0.44	0.49	0.00
	8	-0.42	-0.27	0.04
	9	-0.10	-0.04	0.01
	10	0.17	0.21	0.01
	11	0.86	0.89	0.00
LiI	1	0.63	0.78	0.02
	2	-0.63	0.22	0.98
Pyrrole/Li ⁺	1	-0.48	-0.38	0.01
	2	0.00	0.19	0.37
	3	0.00	0.19	0.37
	4	0.40	0.41	0.00
	5	-0.14	-0.04	0.10
	6	0.16	0.20	0.02
	7	-0.14	-0.04	0.10
	8	0.16	0.20	0.02
	9	0.14	0.16	0.00
	10	0.14	0.16	0.00

	11	0.74	0.95	0.00
LiBOB	1	0.32	0.43	0.14
	2	0.32	0.43	0.14
	3	0.34	0.36	0.00
	4	0.34	0.36	0.00
	5	0.32	0.36	0.01
	6	-0.23	-0.23	0.00
	7	-0.23	-0.23	0.00
	8	-0.27	-0.17	0.09
	9	-0.27	-0.17	0.09
	10	-0.33	-0.15	0.26
	11	-0.33	-0.15	0.26
	12	-0.36	-0.31	0.00
	13	-0.36	-0.31	0.00
	14	0.76	0.78	0.00
LiDFOB	1	0.33	0.42	0.15
	2	0.33	0.42	0.15
	3	-0.38	-0.16	0.25
	4	-0.38	-0.16	0.25
	5	-0.20	-0.13	0.09
	6	-0.20	-0.13	0.09
	7	-0.18	-0.12	0.00
	8	-0.18	-0.16	0.00

	9	0.08	0.15	0.01
	10	0.76	0.89	0.00

Table S3. CM5 partial charges and spin density values of electrolyte complexes with TFSI⁻
(orders coincide with atom numbers in Figure 4)

Complex		Partial Charge (e)		Spin Density
		Initial State	Oxidized State	Oxidized State
DME_ttt/TFSI ⁻	1	-0.15	-0.12	0.01
	2	0.10	0.12	0.00
	3	0.09	0.11	0.01
	4	0.09	0.11	0.01
	5	-0.31	-0.24	0.19
	6	-0.07	-0.01	0.53
	7	0.10	0.12	0.05
	8	0.10	0.29	0.06
	9	-0.07	-0.07	0.05
	10	0.10	0.11	0.01
	11	0.10	0.11	0.03
	12	-0.31	-0.30	0.01
	13	-0.14	-0.14	0.00
	14	0.10	0.09	0.00
	15	0.11	0.11	0.00
	16	0.10	0.10	0.00
	17	-0.19	-0.23	0.04
	18	0.46	0.54	0.00
	19	0.47	0.54	0.00

	20	-0.40	-0.35	0.00
	21	-0.40	-0.35	0.00
	22	-0.40	-0.35	0.00
	23	-0.41	-0.35	0.00
	24	0.17	0.19	0.00
	25	0.17	0.19	0.00
	26	-0.07	-0.04	0.00
	27	-0.07	-0.03	0.00
	28	-0.07	-0.03	0.00
	29	-0.07	-0.05	0.00
	30	-0.07	-0.04	0.00
	31	-0.07	-0.04	0.00
DME_tgt/TFSI-	1	-0.06	-0.07	0.04
	2	0.10	0.09	0.01
	3	0.10	0.10	0.00
	4	-0.06	0.00	0.52
	5	0.10	0.11	0.04
	6	0.11	0.30	0.06
	7	-0.31	-0.22	0.21
	8	-0.31	-0.30	0.03
	9	-0.14	-0.11	0.01
	10	0.10	0.09	0.01
	11	0.11	0.12	0.00

	12	0.10	0.11	0.01
	13	-0.14	-0.13	0.01
	14	0.10	0.09	0.00
	15	0.11	0.11	0.00
	16	0.10	0.09	0.00
	17	-0.20	-0.47	0.04
	18	0.46	0.64	0.00
	19	0.46	0.64	0.00
	20	-0.40	-0.33	0.00
	21	-0.41	-0.33	0.00
	22	-0.40	-0.33	0.00
	23	-0.41	-0.33	0.00
	24	0.17	0.35	0.00
	25	0.17	0.35	0.0
	26	-0.07	-0.10	0.00
	27	-0.07	-0.09	0.00
	28	-0.07	-0.10	0.00
	29	-0.07	-0.10	0.00
	30	-0.07	-0.10	0.00
	31	-0.07	-0.10	0.00
DOL/TFSI-	1	-0.06	-0.05	0.01
	2	-0.06	-0.05	0.01
	3	0.04	0.08	0.48

	4	0.11	0.11	0.00
	5	0.11	0.14	0.00
	6	0.11	0.13	0.00
	7	0.12	0.13	0.01
	8	0.13	0.15	0.06
	9	0.11	0.28	0.07
	10	-0.31	-0.25	0.14
	11	-0.30	-0.25	0.15
	12	-0.20	-0.23	0.05
	13	0.46	0.54	0.01
	14	0.46	0.54	0.01
	15	-0.40	-0.35	0.00
	16	-0.41	-0.34	0.00
	17	-0.40	-0.35	0.00
	18	-0.41	-0.35	0.00
	19	0.17	0.19	0.00
	20	0.17	0.19	0.00
	21	-0.07	-0.04	0.00
	22	-0.07	-0.04	0.00
	23	-0.07	-0.04	0.00
	24	-0.07	-0.04	0.00
	25	-0.07	-0.04	0.00
	26	-0.07	-0.04	0.00

EDOT/TFSI-	1	-0.17	-0.07	0.22
	2	0.06	0.18	0.20
	3	0.06	0.10	0.04
	4	-0.17	-0.11	0.03
	5	0.04	0.27	0.25
	6	0.13	0.17	0.01
	7	0.13	0.16	0.00
	8	-0.25	-0.22	0.02
	9	-0.25	-0.14	0.19
	10	-0.06	-0.04	0.00
	11	0.11	0.12	0.00
	12	0.12	0.15	0.00
	13	-0.06	-0.03	0.01
	14	0.12	0.15	0.00
	15	0.11	0.15	0.01
	16	-0.18	-0.19	0.01
	17	0.47	0.47	0.00
	18	0.46	0.47	0.00
	19	-0.40	-0.39	0.00
	20	-0.41	-0.39	0.00
	21	-0.40	-0.39	0.00
	22	-0.39	-0.39	0.00
	23	0.17	0.17	0.00

	24	0.17	0.17	0.00
	25	-0.07	-0.06	0.00
	26	-0.07	-0.06	0.00
	27	-0.06	-0.06	0.00
	28	-0.07	-0.06	0.00
	29	-0.07	-0.07	0.00
	30	-0.07	-0.06	0.00
FEC/TFSI-	1	0.09	0.11	0.00
	2	-0.05	-0.03	0.00
	3	0.14	0.15	0.00
	4	0.13	0.15	0.00
	5	-0.22	-0.20	0.00
	6	-0.21	-0.20	0.00
	7	0.38	0.40	0.00
	8	-0.37	-0.31	0.07
	9	-0.12	-0.11	0.00
	10	0.13	0.16	0.00
	11	-0.19	-0.01	0.66
	12	0.47	0.52	0.03
	13	0.47	0.53	0.03
	14	-0.40	-0.33	0.08
	15	-0.40	-0.33	0.02
	16	-0.40	-0.33	0.08

	17	-0.40	-0.33	0.02
	18	0.17	0.19	0.00
	19	0.17	0.20	0.00
	20	-0.07	-0.04	0.00
	21	-0.07	-0.03	0.00
	22	-0.06	-0.04	0.00
	23	-0.06	-0.04	0.00
	24	-0.07	-0.03	0.00
	25	-0.07	-0.04	0.00
Pyrrole/TFSI ⁻	1	-0.46	-0.41	0.01
	2	-0.03	0.17	0.37
	3	-0.03	0.17	0.37
	4	0.31	0.33	0.00
	5	-0.18	-0.05	0.10
	6	0.13	0.18	0.02
	7	-0.18	-0.05	0.10
	8	0.12	0.19	0.02
	9	0.10	0.15	0.00
	10	0.10	0.15	0.00
	11	-0.19	-0.19	0.00
	12	0.47	0.47	0.00
	13	0.47	0.47	0.00
	14	-0.39	-0.39	0.00

	15	-0.40	-0.39	0.00
	16	-0.38	-0.39	0.00
	17	-0.40	-0.39	0.00
	18	0.17	0.17	0.00
	19	0.17	0.17	0.00
	20	-0.07	-0.06	0.00
	21	-0.07	-0.06	0.00
	22	-0.06	-0.06	0.00
	23	-0.06	-0.06	0.00
	24	-0.07	-0.06	0.00
	25	-0.07	-0.06	0.00

Table S4. CM5 partial charges and spin density values of electrolyte complexes with LiTFSI
(orders coincide with atom numbers in Figure 5)

Complex		Partial Charge (e)		Spin Density
		Initial State	Oxidized State	Oxidized State
DME_ttt/LiTFSI	1	-0.11	-0.12	0.00
	2	0.13	0.12	0.00
	3	0.12	0.12	0.00
	4	0.12	0.12	0.00
	5	-0.36	-0.36	0.01
	6	-0.05	-0.05	0.06
	7	0.12	0.12	0.04
	8	0.12	0.13	0.01
	9	-0.05	0.00	0.64
	10	0.12	0.13	0.05
	11	0.12	0.38	0.00
	12	-0.30	-0.30	0.16
	13	-0.13	-0.11	0.01
	14	0.10	0.12	0.01
	15	0.11	0.13	0.00
	16	0.10	0.12	0.01
	17	0.17	0.28	0.01
	18	-0.17	-0.14	0.00

	19	-0.17	-0.14	0.00
	20	0.59	0.63	0.00
	21	-0.32	-0.34	0.00
	22	0.43	0.50	0.00
	23	-0.37	-0.32	0.00
	24	0.19	0.20	0.00
	25	-0.05	-0.02	0.00
	26	-0.05	-0.03	0.00
	27	-0.05	-0.02	0.00
	28	-0.37	-0.32	0.00
	29	0.18	0.20	0.00
	30	-0.05	-0.02	0.00
	31	-0.05	-0.03	0.00
	32	-0.05	-0.02	0.00
DME_tgt/LiTFSI	1	-0.05	0.00	0.64
	2	0.13	0.13	0.05
	3	0.12	0.38	0.00
	4	-0.05	-0.05	0.06
	5	0.13	0.13	0.01
	6	0.12	0.13	0.04
	7	-0.34	-0.36	0.01
	8	-0.34	-0.30	0.16

	9	-0.12	-0.12	0.00
	10	0.11	0.12	0.00
	11	0.13	0.12	0.00
	12	0.11	0.12	0.00
	13	-0.12	-0.11	0.01
	14	0.11	0.12	0.01
	15	0.13	0.13	0.00
	16	0.11	0.12	0.01
	17	0.18	0.27	0.02
	18	-0.17	-0.14	0.00
	19	-0.17	-0.14	0.00
	20	0.58	0.63	0.00
	21	-0.32	-0.34	0.00
	22	0.43	0.51	0.00
	23	-0.38	-0.32	0.00
	24	0.18	0.20	0.00
	25	-0.06	-0.02	0.00
	26	-0.05	-0.03	0.00
	27	-0.05	-0.02	0.00
	28	-0.38	-0.32	0.00
	29	0.18	0.20	0.00
	30	-0.05	-0.01	0.00

	31	-0.05	-0.03	0.00
	32	-0.05	-0.02	0.00
DOL/LiTFSI	1	-0.04	-0.04	0.01
	2	-0.05	-0.04	0.01
	3	0.06	0.07	0.62
	4	0.13	0.15	0.00
	5	0.13	0.13	0.00
	6	0.12	0.13	0.01
	7	0.13	0.14	0.00
	8	0.15	0.38	0.00
	9	0.13	0.15	0.06
	10	-0.35	-0.33	0.11
	11	-0.28	-0.24	0.16
	12	0.20	0.30	0.01
	13	-0.17	-0.14	0.00
	14	-0.18	-0.14	0.00
	15	0.59	0.64	0.00
	16	-0.32	-0.34	0.00
	17	0.43	0.51	0.00
	18	-0.37	-0.31	0.00
	19	0.18	0.21	0.00
	20	-0.05	-0.02	0.00

	21	-0.05	-0.02	0.00
	22	-0.05	-0.02	0.00
	23	-0.37	-0.31	0.00
	24	0.18	0.21	0.00
	25	-0.05	-0.02	0.00
	26	-0.05	-0.02	0.00
	27	-0.05	-0.02	0.00
EDOT/LiTFSI	1	-0.13	-0.03	0.27
	2	0.07	0.19	0.20
	3	0.07	0.11	0.01
	4	-0.11	-0.07	0.08
	5	0.02	0.29	0.20
	6	0.13	0.19	0.01
	7	0.14	0.18	0.00
	8	-0.29	-0.26	0.00
	9	-0.23	-0.13	0.20
	10	-0.03	-0.02	0.00
	11	0.13	0.15	0.00
	12	0.14	0.16	0.00
	13	-0.04	-0.01	0.01
	14	0.14	0.17	0.00
	15	0.12	0.16	0.01

	16	0.63	0.20	0.00
	17	-0.44	-0.18	0.00
	18	-0.44	-0.18	0.00
	19	0.63	0.59	0.00
	20	-0.46	-0.32	0.00
	21	0.63	0.43	0.00
	22	-0.36	-0.37	0.00
	23	-0.36	-0.37	0.00
	24	0.35	0.19	0.00
	25	-0.10	-0.05	0.00
	26	-0.11	-0.05	0.00
	27	-0.11	-0.05	0.00
	28	0.35	0.19	0.00
	29	-0.11	-0.05	0.00
	30	-0.10	-0.05	0.00
	31	-0.10	-0.04	0.00
FEC/LiTFSI	1	0.17	0.11	0.00
	2	-0.01	-0.02	0.00
	3	0.15	0.16	0.00
	4	0.15	0.16	0.00
	5	-0.17	-0.18	0.00
	6	-0.18	-0.18	0.00

	7	0.41	0.44	0.00
	8	-0.38	-0.41	0.00
	9	-0.16	-0.10	0.00
	10	0.16	0.17	0.00
	11	0.63	0.36	0.00
	12	-0.43	-0.13	0.08
	13	-0.44	-0.13	0.08
	14	0.63	0.61	0.03
	15	-0.47	-0.09	0.71
	16	0.63	0.50	0.04
	17	-0.36	-0.30	0.04
	18	0.35	0.21	0.00
	19	-0.10	-0.02	0.00
	20	-0.11	-0.02	0.00
	21	-0.11	-0.02	0.00
	22	-0.36	-0.29	0.02
	23	0.35	0.21	0.00
	24	-0.11	-0.01	0.00
	25	-0.11	-0.02	0.00
	26	-0.10	-0.01	0.00
F/LiTFSI	1	0.42	0.54	0.02
	2	-0.66	0.21	0.98

	3	-0.43	-0.44	0.00
	4	-0.43	-0.44	0.00
	5	0.62	0.63	0.00
	6	-0.47	-0.46	0.00
	7	0.62	0.63	0.00
	8	-0.37	-0.36	0.00
	9	-0.37	-0.36	0.00
	10	0.35	0.35	0.00
	11	-0.11	-0.11	0.00
	12	-0.11	-0.10	0.00
	13	-0.10	-0.10	0.00
	14	0.34	0.35	0.00
	15	-0.10	-0.10	0.00
	16	-0.11	-0.10	0.00
	17	-0.11	-0.11	0.00
Pyrrole/LiTFSI	1	-0.43	-0.39	0.01
	2	0.00	0.19	0.37
	3	0.00	0.18	0.37
	4	0.38	0.41	0.00
	5	-0.14	-0.03	0.10
	6	0.15	0.20	0.02
	7	-0.14	-0.04	0.10

	8	0.15	0.20	0.02
	9	0.13	0.17	0.00
	10	0.13	0.17	0.00
	11	0.53	0.25	0.00
	12	-0.43	-0.18	0.00
	13	-0.43	-0.18	0.00
	14	0.62	0.60	0.00
	15	-0.47	-0.31	0.00
	16	0.62	0.44	0.00
	17	-0.36	-0.37	0.00
	18	0.35	0.19	0.00
	19	-0.10	-0.05	0.00
	20	-0.11	-0.05	0.00
	21	-0.11	-0.05	0.00
	22	-0.37	-0.37	0.00
	23	0.35	0.19	0.00
	24	-0.11	-0.05	0.00
	25	-0.11	-0.05	0.00
	26	-0.10	-0.05	0.00
BOB-/LiTFSI	1	0.32	0.43	0.14
	2	0.32	0.43	0.14
	3	0.34	0.36	0.00

	4	0.34	0.36	0.00
	5	0.31	0.36	0.01
	6	-0.24	-0.24	0.00
	7	-0.24	-0.24	0.00
	8	-0.27	-0.17	0.09
	9	-0.27	-0.17	0.09
	10	-0.34	-0.15	0.26
	11	-0.34	-0.15	0.26
	12	-0.35	-0.30	0.00
	13	-0.35	-0.30	0.00
	14	0.14	0.13	0.00
	15	-0.17	-0.16	0.00
	16	0.51	0.51	0.00
	17	0.51	0.51	0.00
	18	-0.26	-0.26	0.00
	19	-0.38	-0.37	0.00
	20	-0.26	-0.26	0.00
	21	-0.38	-0.37	0.00
	22	0.18	0.18	0.00
	23	0.18	0.18	0.00
	24	-0.05	-0.05	0.00
	25	-0.06	-0.05	0.00
	26	-0.05	-0.05	0.00

	27	-0.05	-0.04	0.00
	28	-0.06	-0.05	0.00
	29	-0.05	-0.05	0.00
DFOB-/LiTFSI	1	0.33	0.38	0.15
	2	0.33	0.37	0.15
	3	-0.36	-0.16	0.25
	4	-0.36	-0.16	0.25
	5	-0.21	-0.12	0.09
	6	-0.21	-0.12	0.09
	7	-0.19	-0.13	0.00
	8	-0.19	-0.15	0.00
	9	0.08	0.12	0.01
	10	0.15	0.65	0.00
	11	-0.17	-0.46	0.00
	12	-0.17	0.63	0.00
	13	0.58	0.63	0.00
	14	-0.33	-0.43	0.00
	15	0.43	-0.35	0.00
	16	-0.38	-0.44	0.00
	17	-0.38	-0.36	0.00
	18	0.18	0.35	0.00
	19	-0.05	0.35	0.00
	20	-0.06	-0.10	0.00

	21	-0.05	-0.10	0.00
	22	0.18	-0.10	0.00
	23	-0.04	-0.10	0.00
	24	-0.06	-0.10	0.00
	25	-0.05	-0.10	0.00

Table S5. CM5 partial charges and spin density values of electrolyte complexes with S₈ (orders coincide with atom numbers in Figure 6)

Complex		Partial Charge (e)		Spin Density
		Initial State	Oxidized State	Oxidized State
DME_ttt/S ₈	1	-0.13	-0.09	0.01
	2	0.10	0.13	0.02
	3	0.09	0.12	0.01
	4	0.09	0.13	0.00
	5	-0.30	-0.17	0.24
	6	-0.06	0.02	0.17
	7	0.08	0.15	0.02
	8	0.09	0.15	0.02
	9	-0.06	0.03	0.17
	10	0.10	0.16	0.02
	11	0.09	0.15	0.02
	12	-0.28	-0.16	0.25
	13	-0.13	-0.08	0.01
	14	0.09	0.13	0.02
	15	0.10	0.13	0.00
	16	0.09	0.14	0.00
	17	-0.01	0.00	0.00
	18	-0.01	0.01	0.00
	19	0.00	0.01	0.00

	20	-0.01	0.01	0.00
	21	0.02	0.01	0.00
	22	0.01	0.00	0.00
	23	0.02	0.01	0.00
	24	-0.01	0.00	0.00
DME_tgt/S ₈	1	-0.05	0.03	0.16
	2	0.10	0.16	0.03
	3	0.10	0.16	0.02
	4	-0.06	0.02	0.16
	5	0.10	0.16	0.02
	6	0.09	0.15	0.02
	7	-0.29	-0.16	0.25
	8	-0.28	-0.16	0.25
	9	-0.13	-0.09	0.02
	10	0.09	0.12	0.01
	11	0.10	0.14	0.01
	12	0.08	0.13	0.02
	13	-0.13	-0.09	0.01
	14	0.09	0.13	0.01
	15	0.10	0.14	0.00
	16	0.09	0.13	0.00
	17	-0.01	0.00	0.00
	18	-0.01	0.00	0.00

	19	-0.02	0.00	0.00
	20	0.02	0.01	0.00
	21	-0.01	0.00	0.00
	22	-0.02	0.00	0.00
	23	0.03	0.01	0.00
	24	0.01	0.01	0.00
DOL/S ₈	1	-0.06	-0.02	0.01
	2	-0.06	-0.02	0.01
	3	0.04	0.12	0.16
	4	0.10	0.13	0.01
	5	0.10	0.15	0.00
	6	0.10	0.14	0.00
	7	0.10	0.14	0.01
	8	0.12	0.19	0.06
	9	0.11	0.13	0.10
	10	-0.28	-0.19	0.16
	11	-0.28	-0.19	0.17
	12	0.02	0.05	0.01
	13	0.01	0.04	0.02
	14	0.02	0.03	0.01
	15	-0.01	0.03	0.00
	16	-0.01	0.13	0.22
	17	-0.01	0.05	0.01

	18	-0.01	0.04	0.02
	19	-0.01	0.03	0.01
FSI/S ₈	1	-0.48	-0.46	0.00
	2	0.69	0.70	0.00
	3	0.69	0.70	0.00
	4	-0.39	-0.37	0.00
	5	-0.39	-0.38	0.00
	6	-0.38	-0.38	0.01
	7	-0.38	-0.37	0.00
	8	-0.16	-0.14	0.00
	9	-0.16	-0.14	0.00
	10	0.01	0.05	0.03
	11	-0.02	0.08	0.05
	12	-0.01	0.16	0.17
	13	-0.01	0.22	0.44
	14	0.00	0.06	0.05
	15	0.01	0.05	0.03
	16	-0.02	0.08	0.06
	17	-0.01	0.16	0.16
TFSI/S ₈	1	-0.49	-0.41	0.19
	2	0.59	0.61	0.01
	3	0.59	0.61	0.01
	4	-0.38	-0.37	0.00

	5	-0.39	-0.36	0.03
	6	-0.39	-0.37	0.00
	7	-0.40	-0.36	0.02
	8	0.33	0.34	0.00
	9	0.33	0.34	0.00
	10	-0.13	-0.11	0.00
	11	-0.13	-0.10	0.00
	12	-0.12	-0.11	0.00
	13	-0.12	-0.12	0.00
	14	-0.13	-0.11	0.00
	15	-0.13	-0.11	0.00
	16	-0.02	0.22	0.49
	17	-0.01	0.09	0.06
	18	-0.01	0.06	0.05
	19	-0.01	0.03	0.02
	20	-0.01	0.09	0.05
	21	0.00	0.06	0.04
	22	0.01	0.03	0.02
	23	-0.02	0.04	0.02
I/S ₈	1	-0.90	-0.11	0.84
	2	-0.01	0.01	0.01
	3	-0.01	0.01	0.01
	4	-0.01	0.01	0.00

	5	-0.02	0.00	0.00
	6	-0.02	0.05	0.10
	7	-0.01	0.01	0.01
	8	-0.01	0.01	0.01
	9	-0.01	0.01	0.00
Pyrrole/S ₈	1	-0.46	-0.39	0.01
	2	-0.01	0.17	0.36
	3	-0.02	0.17	0.36
	4	0.37	0.41	0.00
	5	-0.16	-0.05	0.09
	6	0.13	0.19	0.02
	7	-0.16	-0.05	0.10
	8	0.13	0.19	0.02
	9	0.11	0.16	0.00
	10	0.11	0.16	0.00
	11	0.00	0.00	0.02
	12	0.00	0.00	0.01
	13	-0.01	0.01	0.00
	14	-0.01	0.01	0.00
	15	0.00	0.00	0.00
	16	-0.01	0.01	0.00
	17	-0.01	0.01	0.00
	18	-0.01	0.01	0.00

Table S6. CM5 partial charges and spin density values of electrolyte complexes with pyrene
(orders coincide with atom numbers in Figure 7)

Complex		Partial Charge (e)		Spin Density
		Initial State	Oxidized State	Oxidized State
DME_ttt/Pyrene	1	-0.14	-0.14	0.00
	2	0.11	0.11	0.00
	3	0.10	0.10	0.00
	4	0.10	0.10	0.00
	5	-0.31	-0.31	0.00
	6	-0.06	-0.06	0.00
	7	0.10	0.10	0.00
	8	0.10	0.10	0.00
	9	-0.06	-0.06	0.00
	10	0.10	0.11	0.00
	11	0.10	0.10	0.00
	12	-0.29	-0.29	0.00
	13	-0.14	-0.14	0.00
	14	0.10	0.10	0.00
	15	0.11	0.11	0.00
	16	0.10	0.10	0.00
	17	-0.11	-0.08	-0.02
	18	-0.11	-0.03	0.17
	19	-0.02	0.01	0.02

	20	-0.01	0.00	0.00
	21	-0.02	0.01	0.02
	22	-0.11	-0.03	0.17
	23	-0.10	-0.05	0.07
	24	-0.01	0.00	0.00
	25	-0.02	0.01	0.02
	26	-0.10	-0.05	0.07
	27	-0.11	-0.03	0.16
	28	0.12	0.14	0.01
	29	-0.11	-0.08	-0.02
	30	-0.11	-0.03	0.16
	31	-0.02	0.01	0.02
	32	-0.10	-0.05	0.07
	33	-0.10	-0.05	0.07
	34	0.12	0.14	0.00
	35	0.12	0.14	0.00
	36	0.11	0.13	0.00
	37	0.12	0.14	0.00
	38	0.12	0.14	0.01
	39	0.12	0.14	0.01
	40	0.11	0.13	0.00
	41	0.12	0.14	0.00
	42	0.12	0.14	0.01

DME_tgt/Pyrene	1	-0.06	-0.06	0.00
	2	0.11	0.09	0.00
	3	0.11	0.10	0.00
	4	-0.06	-0.06	0.00
	5	0.11	0.09	0.00
	6	0.11	0.09	0.00
	7	-0.30	-0.29	0.00
	8	-0.28	-0.29	0.00
	9	-0.14	-0.13	0.00
	10	0.10	0.09	0.00
	11	0.11	0.11	0.00
	12	0.09	0.09	0.00
	13	-0.14	-0.13	0.00
	14	0.10	0.08	0.00
	15	0.11	0.10	0.00
	16	0.10	0.09	0.00
	17	-0.11	-0.07	-0.03
	18	-0.11	-0.02	0.17
	19	-0.02	0.01	0.02
	20	-0.01	0.01	0.00
	21	-0.02	0.01	0.01
	22	-0.11	-0.02	0.17
	23	-0.11	-0.04	0.07

	24	-0.01	0.01	0.00
	25	-0.02	0.01	0.02
	26	-0.11	-0.04	0.07
	27	-0.11	-0.02	0.17
	28	0.11	0.14	0.01
	29	-0.11	-0.07	-0.03
	30	-0.11	-0.02	0.17
	31	-0.02	0.01	0.02
	32	-0.11	-0.04	0.07
	33	-0.11	-0.04	0.07
	34	0.11	0.14	0.00
	35	0.11	0.13	0.00
	36	0.12	0.13	0.00
	37	0.11	0.13	0.00
	38	0.11	0.14	0.01
	39	0.10	0.14	0.01
	40	0.12	0.13	0.00
	41	0.11	0.13	0.00
	42	0.11	0.14	0.01
DOL/Pyrene	1	-0.06	-0.06	0.00
	2	-0.06	-0.06	0.00
	3	0.04	0.04	0.00
	4	0.11	0.12	0.00

	5	0.12	0.11	0.00
	6	0.11	0.11	0.00
	7	0.12	0.11	0.00
	8	0.13	0.12	0.00
	9	0.11	0.14	0.00
	10	-0.30	-0.29	0.00
	11	-0.30	-0.29	0.00
	12	-0.11	-0.08	-0.02
	13	-0.11	-0.03	0.16
	14	-0.02	0.01	0.02
	15	-0.01	0.00	0.00
	16	-0.02	0.01	0.02
	17	-0.11	-0.03	0.16
	18	-0.10	-0.05	0.07
	19	-0.01	0.00	0.00
	20	-0.02	0.01	0.02
	21	-0.10	-0.05	0.07
	22	-0.11	-0.03	0.16
	23	0.12	0.14	0.01
	24	-0.11	-0.08	-0.02
	25	-0.11	-0.03	0.16
	26	-0.02	0.01	0.02
	27	-0.10	-0.05	0.07

	28	-0.10	-0.05	0.07
	29	0.12	0.14	0.00
	30	0.12	0.14	0.00
	31	0.12	0.14	0.00
	32	0.12	0.14	0.00
	33	0.12	0.14	0.01
	34	0.12	0.14	0.01
	35	0.12	0.14	0.00
	36	0.12	0.12	0.00
	37	0.12	0.13	0.01
FSI/Pyrene	1	-0.46	-0.17	0.00
	2	0.70	0.55	0.00
	3	0.70	0.55	0.00
	4	-0.39	-0.39	0.00
	5	-0.38	-0.39	0.00
	6	-0.38	-0.39	0.00
	7	-0.39	-0.39	0.00
	8	-0.16	-0.14	0.00
	9	-0.16	-0.14	0.00
	10	-0.11	-0.08	-0.02
	11	-0.10	-0.03	0.16
	12	-0.02	0.01	0.01
	13	-0.01	0.00	0.00

	14	-0.02	0.01	0.01
	15	-0.10	-0.03	0.16
	16	-0.10	-0.05	0.07
	17	-0.01	0.00	0.00
	18	-0.02	0.01	0.02
	19	-0.10	-0.05	0.06
	20	-0.10	-0.03	0.16
	21	0.11	0.14	0.01
	22	-0.11	-0.08	-0.02
	23	-0.10	-0.03	0.17
	24	-0.02	0.01	0.02
	25	-0.10	-0.05	0.06
	26	-0.10	-0.05	0.08
	27	0.11	0.14	0.00
	28	0.11	0.14	0.00
	29	0.11	0.14	0.00
	30	0.11	0.13	0.00
	31	0.11	0.14	0.01
	32	0.11	0.14	0.01
	33	0.11	0.14	0.00
	34	0.09	0.12	0.00
	35	0.09	0.12	0.01
TFSI-/Pyrene	1	-0.20	-0.19	0.00

	2	0.46	0.47	0.00
	3	0.46	0.47	0.00
	4	-0.40	-0.40	0.00
	5	-0.41	-0.39	0.00
	6	-0.40	-0.41	0.00
	7	-0.41	-0.40	0.00
	8	0.17	0.17	0.00
	9	0.17	0.17	0.00
	10	-0.07	-0.07	0.00
	11	-0.07	-0.07	0.00
	12	-0.07	-0.07	0.00
	13	-0.07	-0.06	0.00
	14	-0.07	-0.07	0.00
	15	-0.07	-0.07	0.00
	16	-0.11	-0.08	-0.02
	17	-0.11	-0.03	0.17
	18	-0.02	0.01	0.02
	19	-0.01	0.00	0.00
	20	-0.02	0.01	0.02
	21	-0.11	-0.03	0.16
	22	-0.11	-0.05	0.07
	23	-0.01	0.00	0.00
	24	-0.02	0.01	0.01

	25	-0.10	-0.05	0.08
	26	-0.10	-0.03	0.17
	27	0.12	0.14	0.01
	28	-0.11	-0.08	-0.02
	29	-0.10	-0.03	0.16
	30	-0.02	0.01	0.01
	31	-0.10	-0.05	0.07
	32	-0.11	-0.05	0.06
	33	0.12	0.14	0.00
	34	0.12	0.14	0.00
	35	0.12	0.13	0.00
	36	0.11	0.13	0.00
	37	0.11	0.12	0.01
	38	0.11	0.14	0.01
	39	0.12	0.14	0.00
	40	0.12	0.13	0.00
	41	0.12	0.14	0.01
I-/Pyrene	1	-0.93	-0.19	0.76
	2	-0.11	-0.11	-0.01
	3	-0.11	-0.10	0.03
	4	-0.02	-0.02	-0.01
	5	-0.01	-0.01	0.00
	6	-0.02	-0.02	0.00

	7	-0.11	-0.10	0.03
	8	-0.11	-0.09	0.03
	9	-0.01	-0.01	-0.01
	10	-0.02	-0.01	0.04
	11	-0.11	-0.10	-0.01
	12	-0.11	-0.10	-0.01
	13	0.11	-0.12	0.00
	14	-0.11	-0.09	0.04
	15	-0.11	-0.07	0.05
	16	-0.02	-0.01	0.04
	17	-0.10	-0.10	0.00
	18	-0.11	-0.09	0.02
	19	0.12	0.12	0.00
	20	0.10	0.12	0.00
	21	0.11	0.12	0.00
	22	0.11	0.12	0.00
	23	0.11	0.12	0.00
	24	0.11	0.12	0.00
	25	0.12	0.12	0.00
	26	0.11	0.12	0.00
	27	0.10	0.12	0.00
Pyrrole/Pyrene	1	-0.42	-0.41	0.00
	2	-0.03	0.02	0.07

	3	-0.03	0.02	0.07
	4	0.36	0.36	0.00
	5	-0.16	-0.13	0.02
	6	0.12	0.13	0.00
	7	-0.17	-0.13	0.02
	8	0.11	0.13	0.00
	9	0.10	0.11	0.00
	10	0.09	0.11	0.00
	11	-0.10	-0.08	-0.02
	12	-0.10	-0.03	0.15
	13	-0.02	0.00	0.02
	14	-0.01	0.00	-0.01
	15	-0.02	0.01	0.03
	16	-0.10	-0.04	0.11
	17	-0.09	-0.05	0.06
	18	-0.01	0.00	0.00
	19	-0.01	0.00	0.00
	20	-0.09	-0.04	0.10
	21	-0.10	-0.04	0.13
	22	0.11	0.13	0.01
	23	-0.10	-0.08	-0.02
	24	-0.10	-0.04	0.14
	25	-0.02	0.00	0.00

	26	-0.10	-0.06	0.05
	27	-0.10	-0.06	0.03
	28	0.11	0.13	0.00
	29	0.11	0.13	0.00
	30	0.11	0.13	0.00
	31	0.11	0.13	0.00
	32	0.11	0.13	0.01
	33	0.11	0.13	0.01
	34	0.11	0.13	0.00
	35	0.11	0.13	0.00
	36	0.11	0.13	0.00

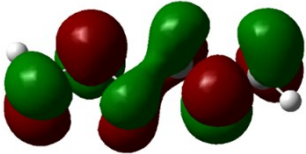
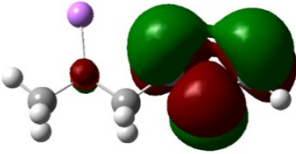
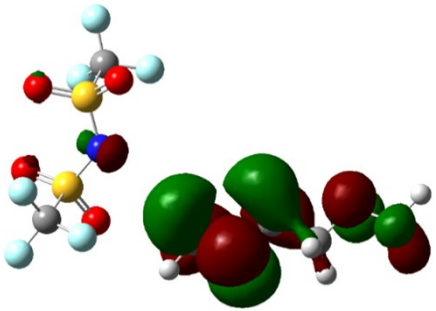
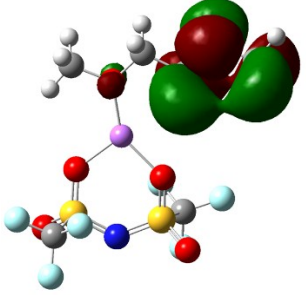
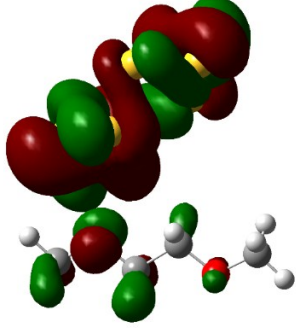
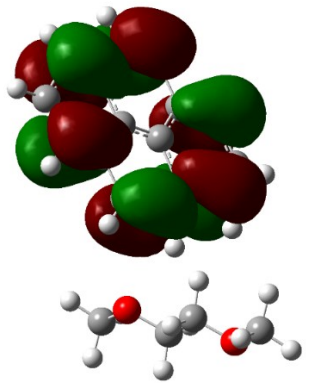
Isolated	Complex with Li ⁺	Complex with TFSI ⁻
		
Complex with LiTFSI	Complex with S ₈	Complex with Pyrene
		

Figure S1. HOMOs of DME_tt in isolated case, and in complexes with Li⁺, TFSI⁻, LiTFSI, S₈, and pyrene.

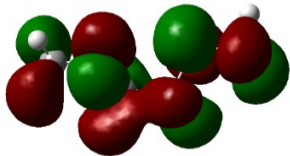
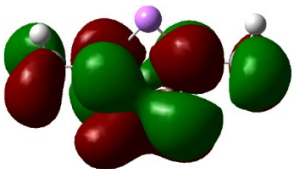
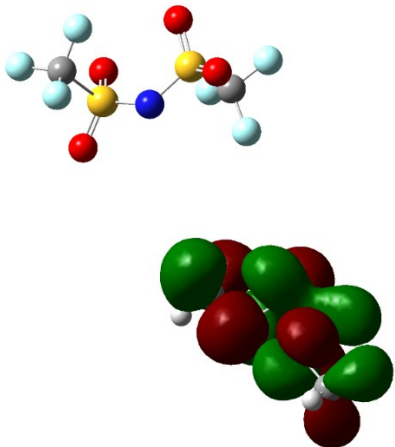
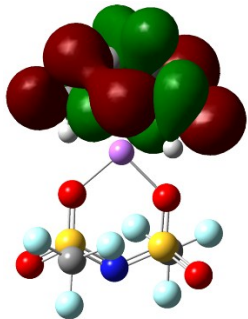
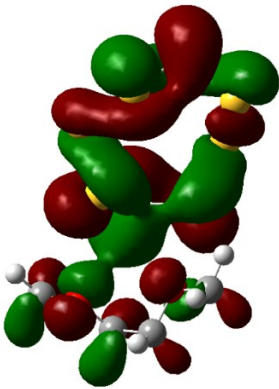
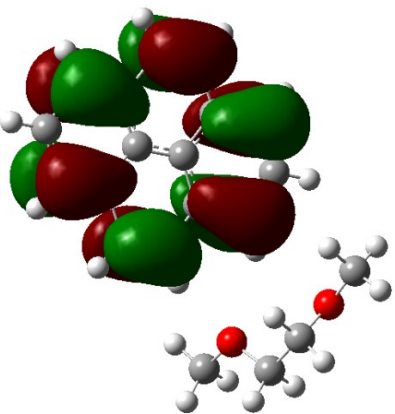
Isolated	Complex with Li^+	Complex with TFSI^-
		
Complex with LiTFSI	Complex with S_8	Complex with Pyrene
		

Figure S2. HOMOs of DME_tgt in isolated case, and in complexes with Li^+ , TFSI^- , LiTFSI , S_8 , and pyrene.

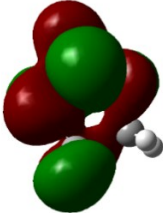
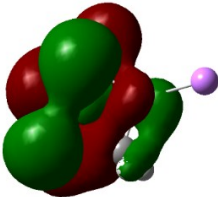
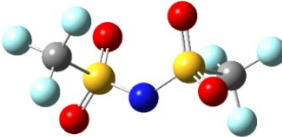
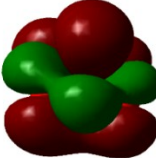
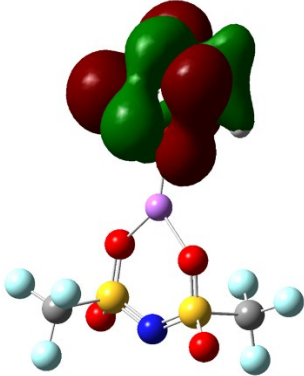
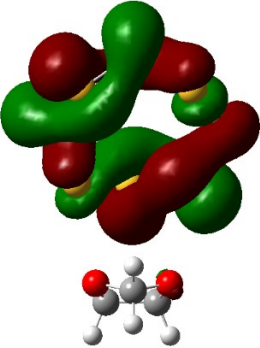
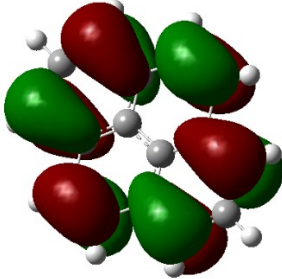
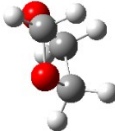
Isolated	Complex with Li ⁺	Complex with TFSI ⁻
		 
Complex with LiTFSI	Complex with S ₈	Complex with Pyrene
		 

Figure S3. HOMOs of DOL in isolated case, and in complexes with Li⁺, TFSI⁻, LiTFSI, S₈, and pyrene.

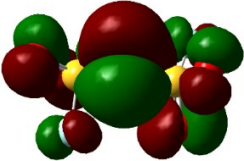
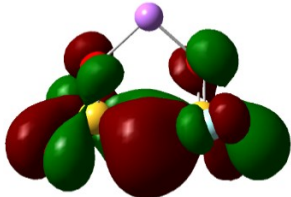
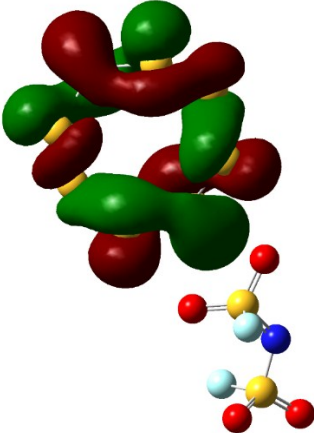
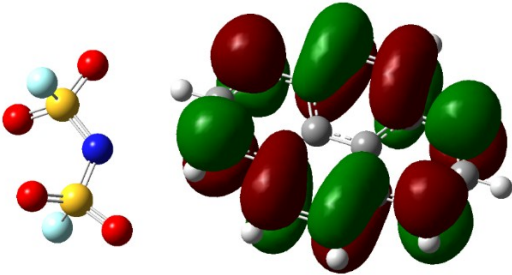
Isolated	Li Salt
	
Complex with S ₈	Complex with Pyrene
	

Figure S4. HOMOs of FSI⁻ in isolated case, and in complexes with Li⁺, S₈, and pyrene.

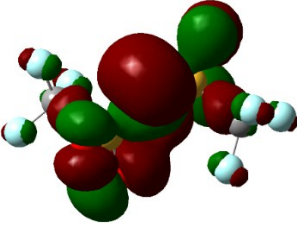
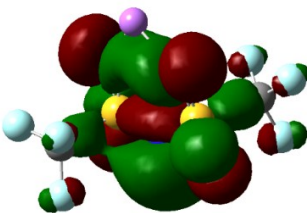
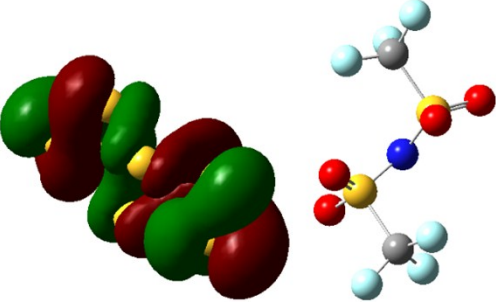
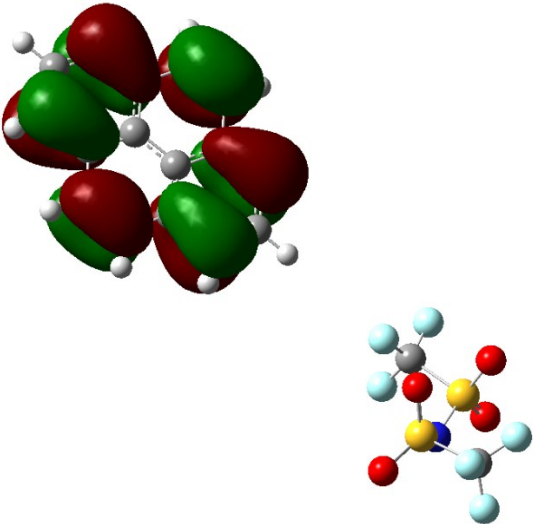
Isolated	Li Salt
	
Complex with S ₈	Complex with Pyrene
	

Figure S5. HOMOs of TFSI⁻ in isolated case, and in complexes with Li⁺, S₈, and pyrene.

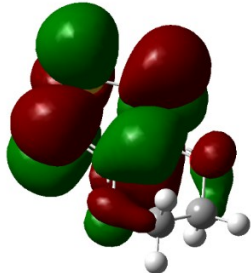
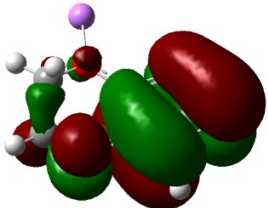
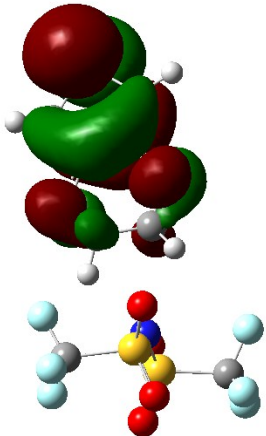
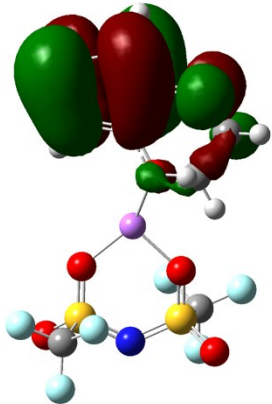
Isolated	Complex with Li^+
	
Complex with TFSI^-	Complex with LiTFSI
	

Figure S6. HOMOs of EDOT in isolated case, and in complexes with Li^+ , and TFSI^- , and LiTFSI .

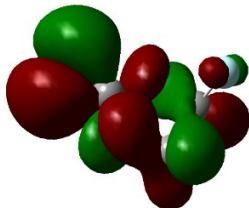
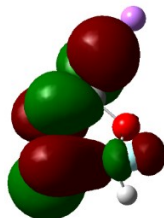
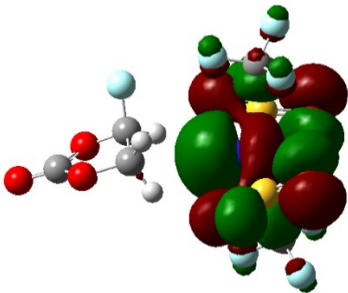
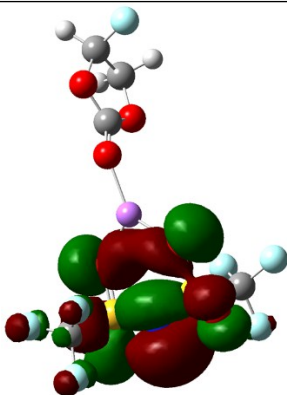
Isolated	Complex with Li ⁺
	
Complex with TFSI ⁻	Complex with LiTFSI
	

Figure S7. HOMOs of FEC in isolated case, and in complexes with Li⁺, and TFSI⁻, and LiTFSI.

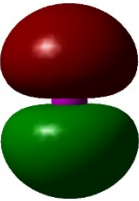
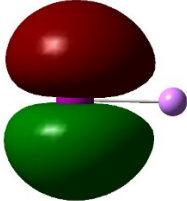
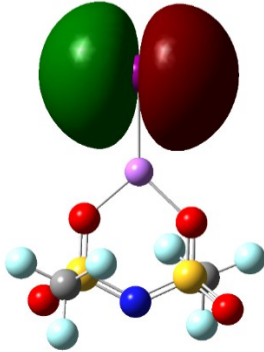
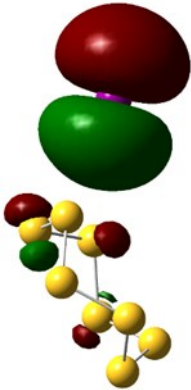
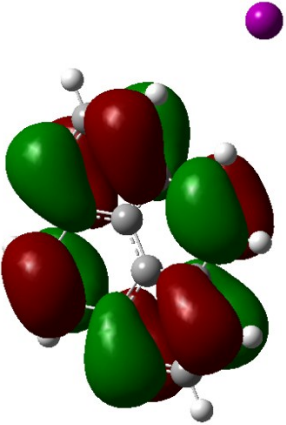
Isolated	Complex with Li^+	Complex with LiTFSI
		
Complex with S_8	Complex with Pyrene	
		

Figure S8. HOMOs of I^- in isolated case, and in complexes with Li^+ , LiTFSI, S_8 , and pyrene.

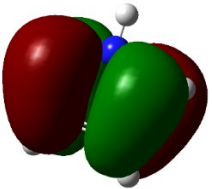
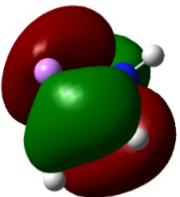
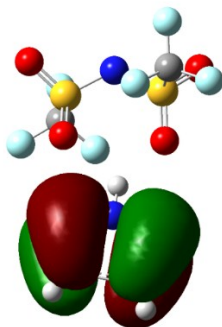
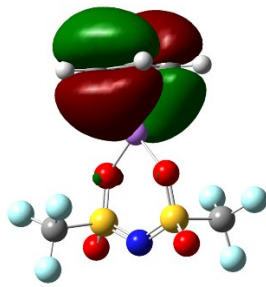
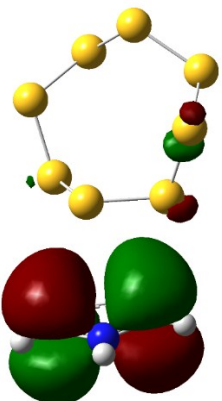
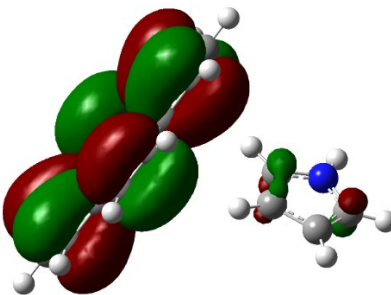
Isolated	Complex with Li^+	Complex with TFSI^-
		
Complex with LiTFSI	Complex with S_8	Complex with Pyrene
		

Figure S9. HOMOs of pyrrole in isolated case, and in complexes with Li^+ , TFSI^- , LiTFSI , S_8 , and pyrene.

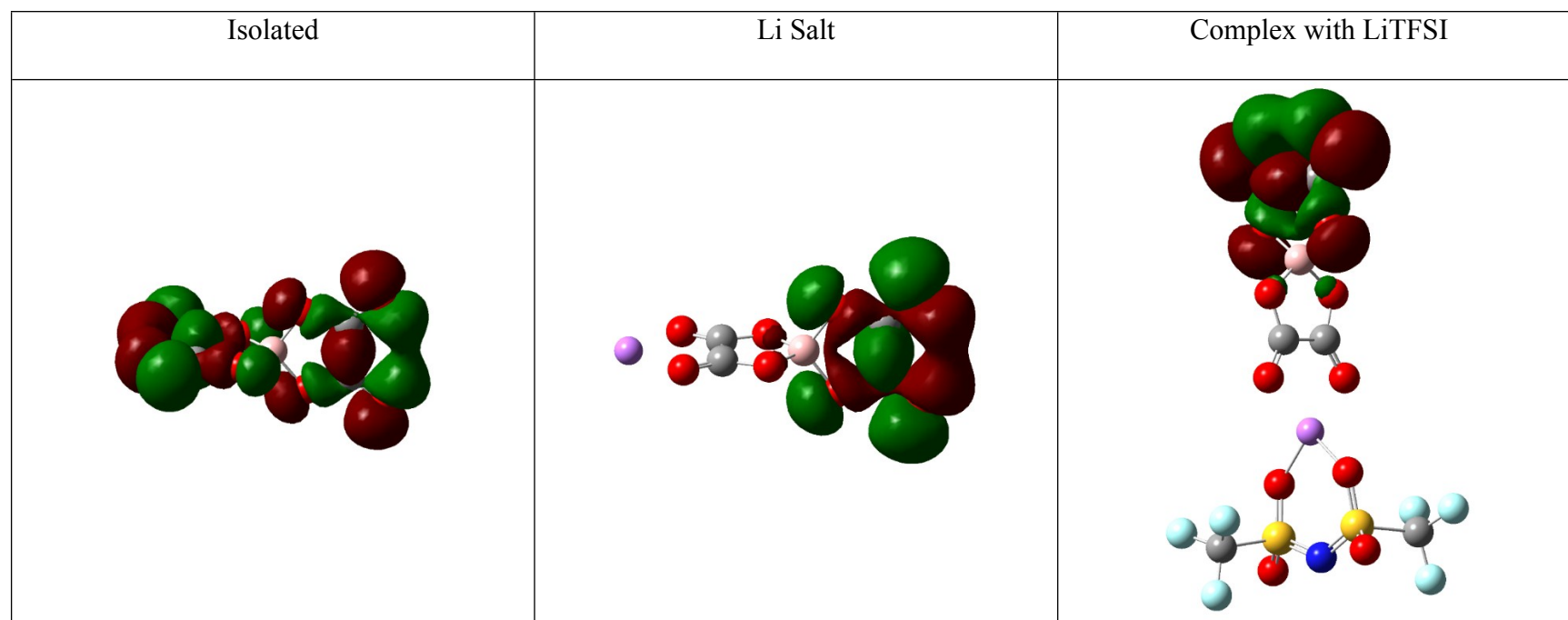


Figure S10. HOMOs of BOB⁻ in isolated case, and in complexes with Li⁺, and LiTFSI.

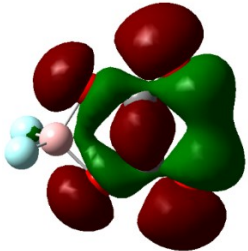
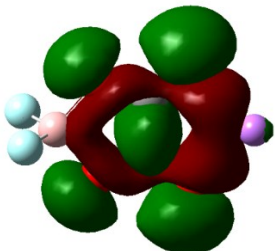
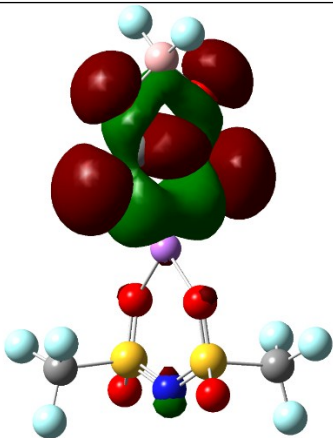
Isolated	Li Salt	Complex with LiTFSI
		

Figure S11. HOMOs of DFOB⁻ in isolated case, and in complexes with Li⁺, and LiTFSI.