SUPPLEMENTARY MATERIAL

Molecular-dynamic simulations

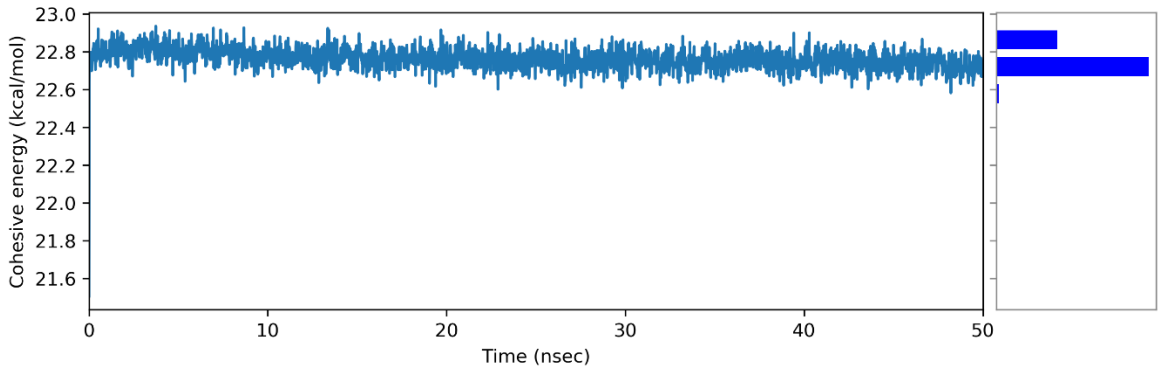

Figure S1. Fluctuations in cohesive energy of 1m $LiBF_4$ (EC/DMC)

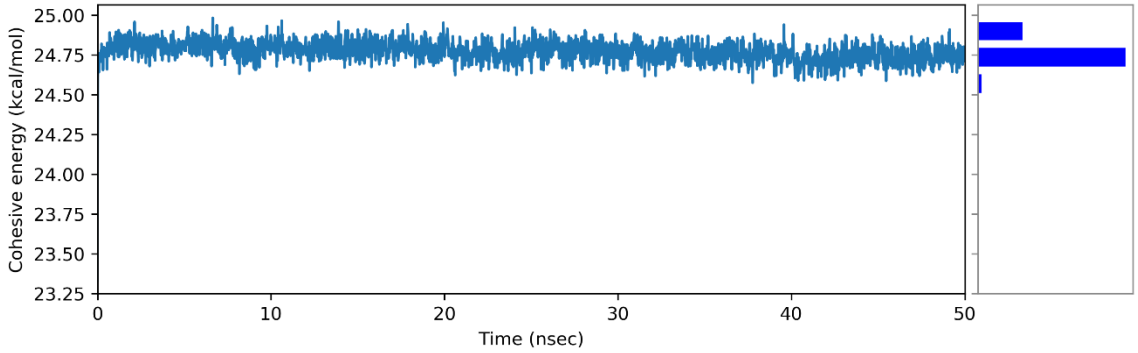

Figure S2. Fluctuations in cohesive energy of 1m LiBF4 (SL/DMC)

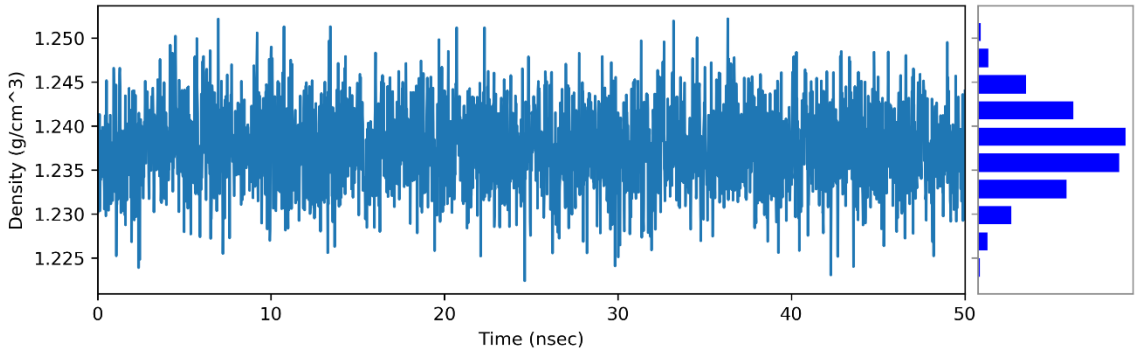

Figure S3. Fluctuation in density value of 1m $LiBF_4$ (EC/DMC)

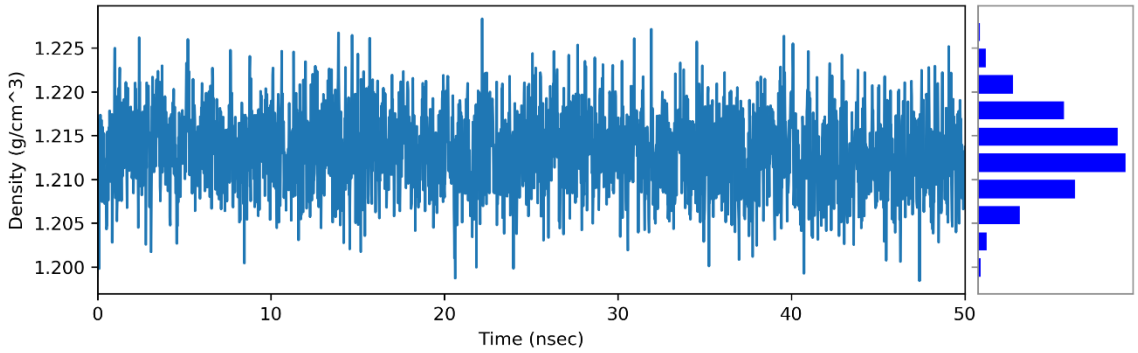

Figure S4. Fluctuation in density value of 1m $LiBF_4$ (SL/DMC)

Quantum-chemical calculations

Table S1. Ionization potential (IP) and electron affinity (EA) values for the all systems, eV.

ID	IP, eV	EA, eV
Solvent or associates		
EC	11.45	-1.09
SL	10.06	-1.92
DMC - 1	10.59	-1.36
DMC - 2	10.39	-1.23
$(DMC)_2$	9.91	-0.97
$(EC)_2$-1	9.95	-0.21
$(EC)_2$-2	8.86	-0.38
$(SL)_2$-1	9.41	0.60
$(SL)_2$-2	9.40	-1.19
$(EC)_1(DMC)_1$-1	10.19	-0.94
$(EC)_1(DMC)_1$-2	10.18	-0.93
$(SL)_1(DMC)_1$-1	9.64	-0.71
$(SL)_1(DMC)_1$-2	9.75	0.17
Solvated anionic complexes		
Non-solvent anion BF_4^-	7,56	-8.48
BF_4^- $(EC)_1$	6.00	
BF_4^- $(DMC)_1$	5.57	
BF_4^- $(SL)_1$	6.76	
BF_4^- $(EC)_2$	6.07	
BF_4^- $(DMC)_2$	5.01	
BF_4^- $(SL)_2$	6.41	
BF_4^- $(EC)_1(DMC)_1$	5.27	

BF_4^- $(SL)_1(DMC)_1$	6.55	-2.88
Solvated cationic complexes		
$Li^+(EC)_1$		3.55
$Li^+(EC)_2$		2.12
$Li^+(EC)_3$		3.15
$Li^+(EC)_4$		3.11
$Li^+(DMC)_1$		3.89
$Li^+(DMC)_2$		2.75
$Li^+(DMC)_3$		2.29
$Li^+(DMC)_4$		2.98
$Li^+(SL)_1$		3.48
$Li^+(SL)_2$		4.72
$Li^+(SL)_3$		1.38
$Li^+(SL)_4$		3.69
$Li^+(EC)_3(DMC)_1$		3.05
$Li^+(EC)_2(DMC)_2$		3.14
$Li^+(EC)_1(DMC)_3$		3.24
$Li^+(SL)_3(DMC)_1$		2.47
$Li^+(SL)_2(DMC)_2$		2.68
$Li^+(SL)_1(DMC)_3$		2.74
$Li^+(EC)_1(DMC)_1$		3.30
$Li^+(EC)_2(DMC)_1$		3.36
$Li^+(EC)_1(DMC)_2$		3.23
$Li^+(SL)_1(DMC)_1$		2.56
$Li^+(SL)_2(DMC)_1$		2.83
$Li^+(SL)_1(DMC)_2$		3.09
Solvated ionic pairs		
Non-solvent ion-pair $\{Li^+BF_4\}$	12.87	0.35
$\{Li^+BF_4\}(EC)_1$	11.99	0.64
$\{Li^+BF_4\}(DMC)_1$	10.00	-0.56
$\{Li^+BF_4\}(EC)_2$	9.31	0.14
$\{Li^+BF_4\}(DMC)_2$	9.68	-0.01
$\{Li^+BF_4\}(EC)_1(DMC)_1$	9.49	-1.05
$\{Li^+BF_4\}(SL)_1$	10.61	-0.47
$\{Li^+BF_4\}(SL)_2$	9.86	0.29
$\{Li^+BF_4\}(SL)_1(DMC)_1$	10.21	1.16

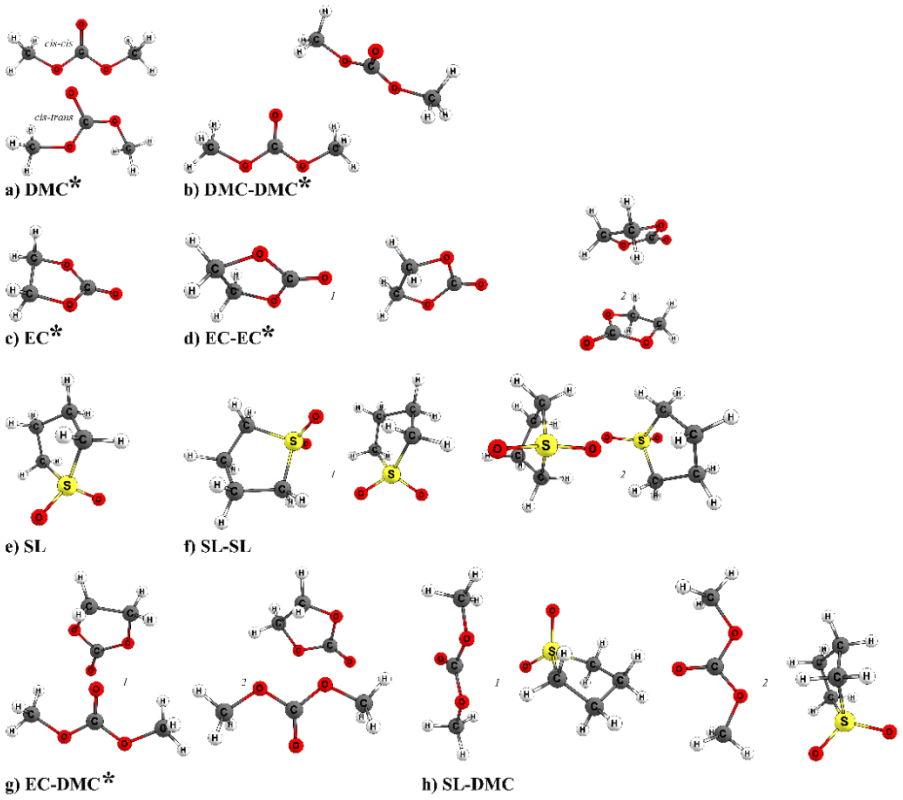

Figure S5. Geometric structure of EC, DMC, SL solvents and their associates

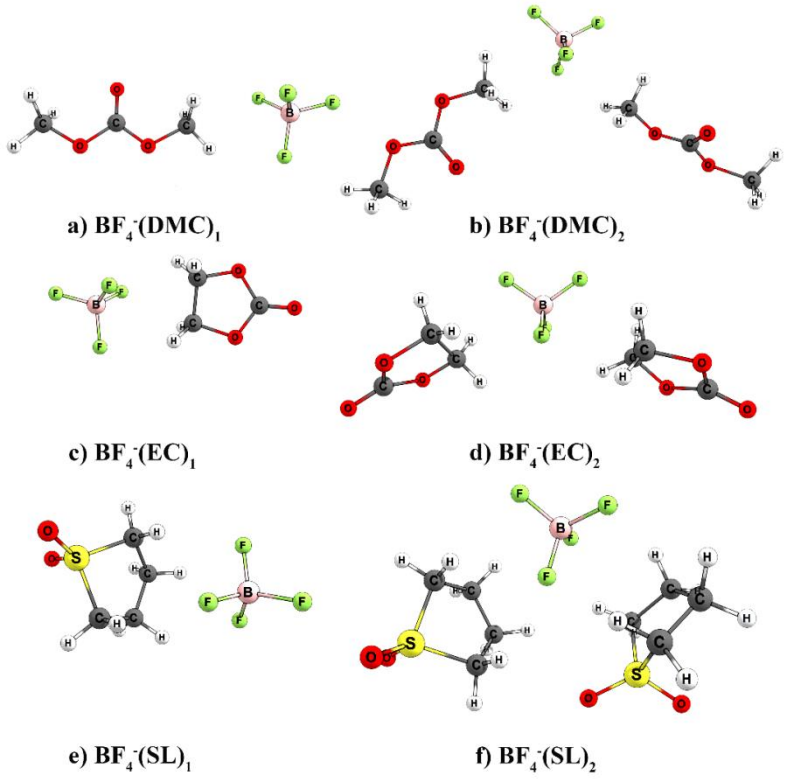

Figure S6. Geometric structure of anionic complexes of the type $BF_4^-(X)_n$, where X=EC, DMC, SL.

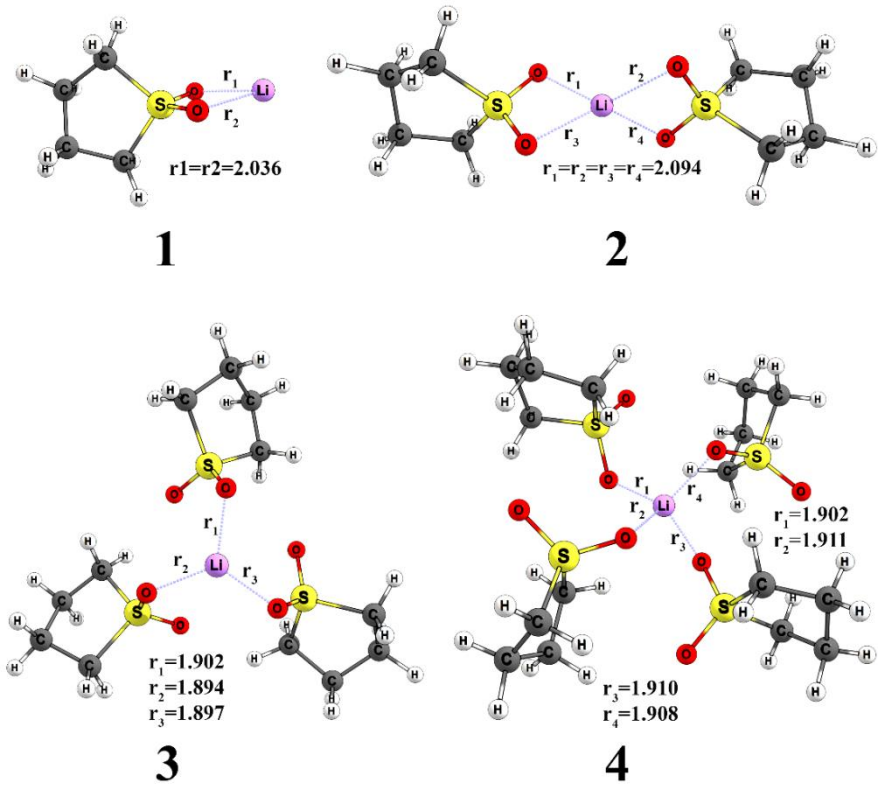

Figure S7. Geometric structure of complexes of the type $Li^{+}SL_n$

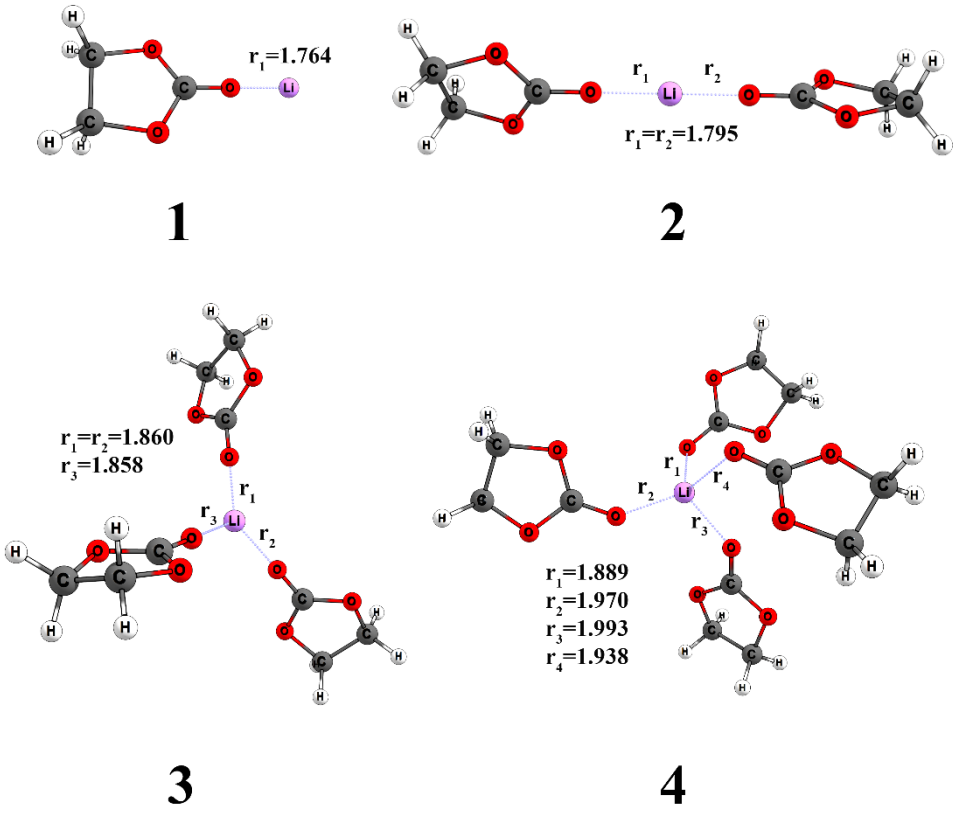

Figure S8. Geometric structure of complexes of the type $Li^{+}EC_n$

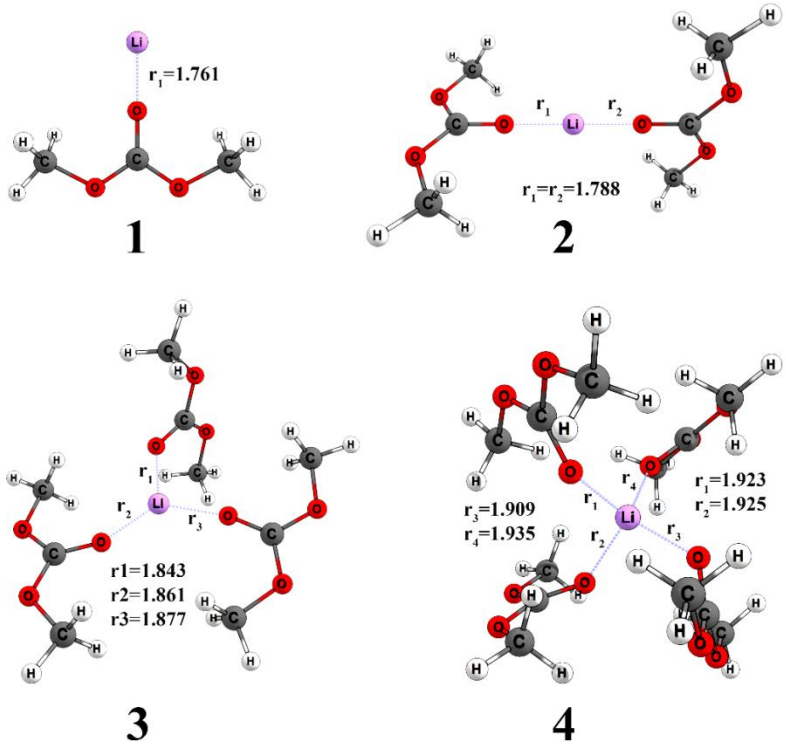

Figure S9. Geometric structure of complexes of the type $Li^{+}DMC_n$

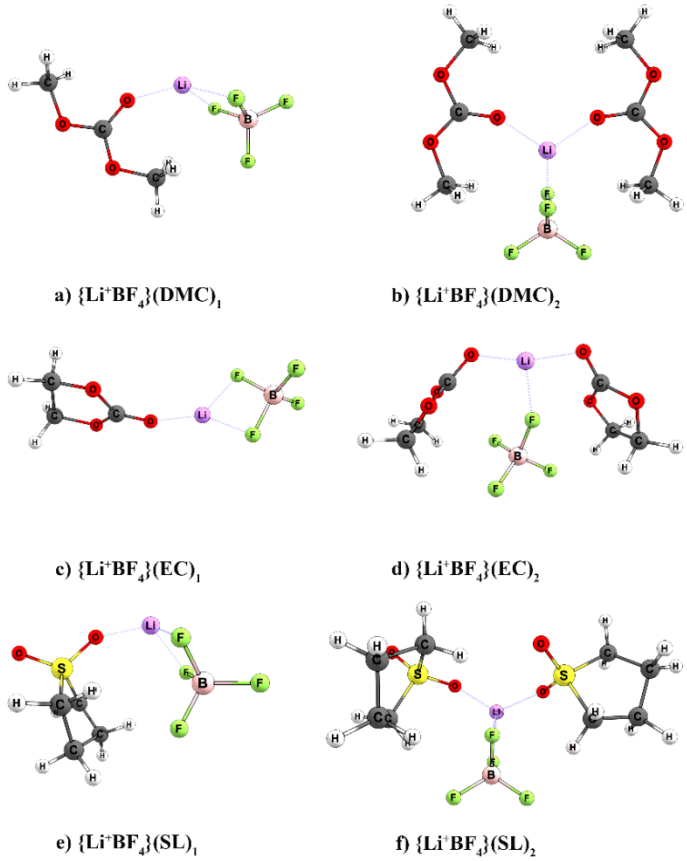

Figure S10. Geometric structure of complexes of the type $\{Li^{+}BF_4\}(X)_n$, where X=EC, DMC, SL.

NMR data

System $LiBF_4$/EC/DMC

1H (δ ppm): 4.33 (4H, s., -CH_2- EC), 3.51 (6H, s., CH_3- DMC)

7Li (δ ppm): -6.68 (s., $\underline{Li}BF_4$)

11B (δ ppm): -7.25 (s., $Li\underline{B}F_4$)

13C (δ ppm): 151.10 (1C, s., $\underline{C}$=O- EC), 150.82 (1C, s., $\underline{C}$=O- DMC), 59.67 (2C, s., CH_2-O-EC), 48.69 (2C, s., CH_3-O- DMC)

17O (δ ppm): 225.5 (1O, br.s., C=$\underline{O}$), 201.6 (1O, w.s., C=$\underline{O}$), 103.8 (2O, br.s., O-CH_2-EC), 84.5 (2O, w.s., O-CH_3- DMC)

19F (δ ppm): -162.04 (s., $Li^{10}BF_4$), -162.09 (s., $Li^{11}BF_4$)

System $LiBF_4$/SL/ DMC

1H (δ ppm): 3.48 (6H, s., CH_3- DMC), 2.78 (4H, m. -CH_2 -S SL), 1.93 (m. -CH_2 - SL),

7Li (δ ppm): -0.11 (s., $\underline{Li}BF_4$)

11B (δ ppm): -1.58 (s., $Li\underline{B}F_4$)

13C (δ ppm): 156.96 (1C, s., DMC), 55.04 (2C, s., CH_2-S- SL), 51.22 (2C, s., CH_3-O-DMC), 22.75 (2C, s., CH_2- SL)

17O (δ ppm): 233.4 (br.s.), 159.3 (w.s.), 90.8 (br.s.)

19F (δ ppm): -155.21 (s., $Li^{10}BF_4$), -155.26 (s., $Li^{11}BF_4$)