SUPPLEMENTARY MATERIAL

Molecular dynamic

Table S 1 Particle ratio in virtual cube

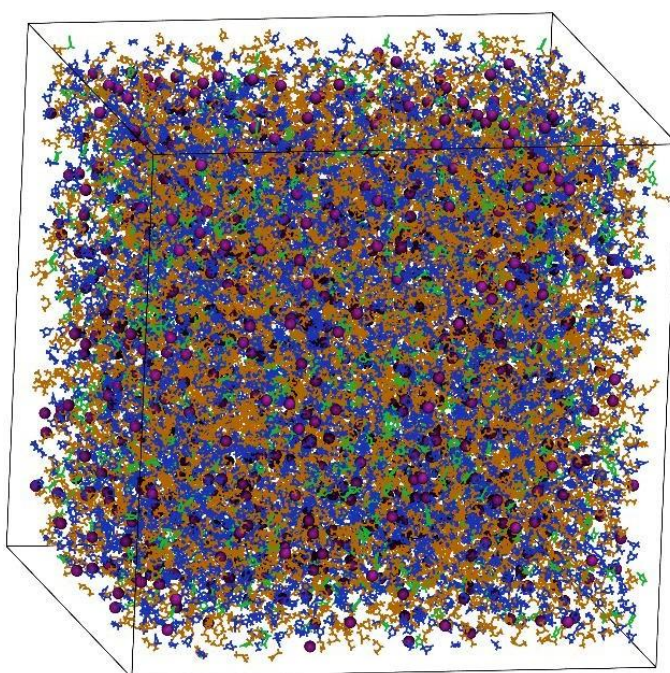| [LiDFOB] mol/kg	Number of molecules	Number of atoms
0.50	24475	256970
0.75	16983	174646
1.00	13237	133485

Figure S 1 Visualization virtual cubes of systems 1m LiDFOB (DMC/EC): lithium cations are shown as violet balls; DFOB− anions – as green molecules, molecules of DMC, EC are shown in blue, and orange colors respectively.
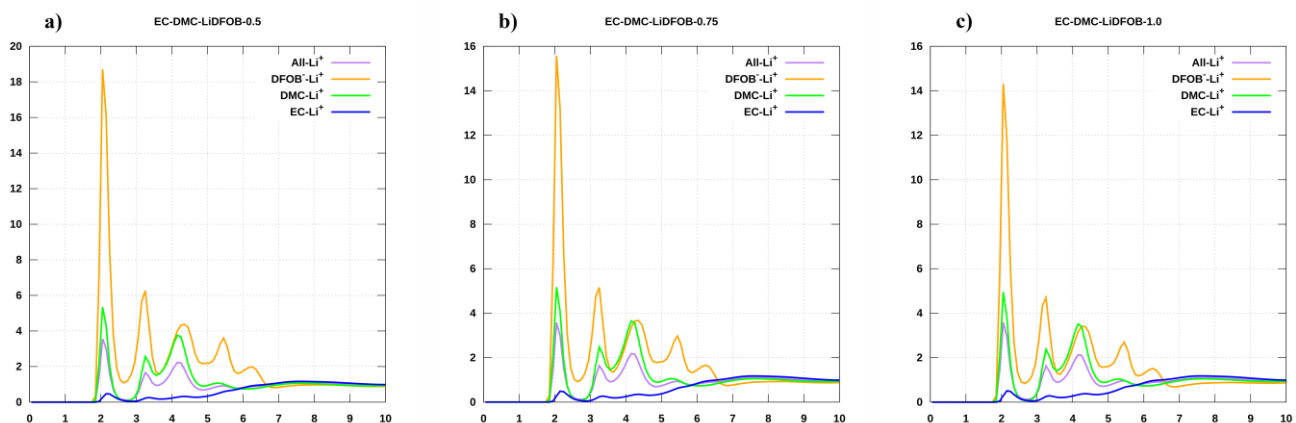

Figure S 2 Radial distribution function.

NMR data

Table S 2 Chemical shifts (ppm) in ^{1}H NMR spectra

[LiDFOB], mol/kg	DMC/EC	
	DMC	EC
0.5	3.57	4.39
0.75	3.56	4.40
1	3.51	4.35

Table S 3 Chemical shifts (ppm) in ^{13}C NMR spectra

[LiDFOB], mol/kg	DMC/EC			
	EC (C̲H$_2$)	EC (C̲O)	DMC (C̲H$_3$)	DMC (C̲O)
0.5	65.2	156.5	54.2	156.4
0.75	65.4	156.8	54.3	156.5
1	66.0	157.4	54.9	157.0

Table S 4 Chemical shifts (ppm) in ^{7}Li, ^{11}B, ^{17}O, ^{19}F NMR spectra

[LiDFOB], mol/kg	EC/DMC			
	^{7}Li	^{11}B	^{19}F	^{17}O
0.5	-0.61	3	-155.7 (^{11}BF̲$_4^-$) -155.6 (^{10}BF̲$_4^-$)	210 (C=O̲, EC),
0.75	-0.59	3	-155.8 (^{11}BF̲$_4^-$) -155.7 (^{10}BF̲$_4^-$)	110 (O̲-, EC), 233 (C=O̲, DMC), 92
1	-0.11	3	-155.4 (^{11}BF̲$_4^-$) -155.3 (^{10}BF̲$_4^-$)	(O̲-,DMC)

Quantum chemistry

Table S 5 Values of the oxidative potential of the complexes

[LiDFOB], mol/kg	Complexes	E^{ox}, V	N, %	E^{ox}_{add}, V	N ($\Delta_f G°$), %	$E^{ox}_{add(form)}$, V	N ($\Delta_f G°_{inc}$), %	$E^{ox}_{add(inc)}$, V
DMC/EC								
0.5	{Li$^+$DFOB$^-$}(DMC)$_1$(EC)$_1$	6.50	69		37		35	
	{Li$^+$(DFOB$^-$)$_2$$^-$}(DMC)$_1(EC)_2$	5.81	19	6.35	28	6.31	30	6.23
	{Li$^+$DFOB$^-$}(DMC)$_2$(EC)$_1$	6.32	12		36		34	
0.75	{Li$^+$DFOB$^-$}(DMC)$_1$(EC)$_1$	6.50	63		36		35	
	{Li$^+$DFOB$^-$}(DMC)$_2$(EC)$_2$	6.31	24	6.44	30	6.41	31	6.40
	{Li$^+$DFOB$^-$}(DMC)$_1$(EC)$_2$	6.39	13		34		34	
1.0	{Li$^+$DFOB$^-$}(DMC)$_1$(EC)$_1$	6.50	24		49		49	
	{Li$^+$DFOB$^-$}(DMC)$_1$(EC)$_2$	6.39	76	6.49	51	6.45	51	6.45