Supporting information

Heterogeneous microstructures and dynamics of the Li-ion electrolyte with fluorinated additive solvent from molecular dynamics simulations

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Table S1. Charge and van der Waals parameter for TFPC solvent

system	Atom	q [e]	σ [Å]	ε [kJ/mol]
TFPC	C1	-0.01778	3.500	2.76144e-01
	C2	0.08135	3.5	2.76144e-01
	H1	0.13285	2.5	1.25520e-01
	H2	0.08792	2.5	1.25520e-01
	H3	0.08792	2.5	1.25520e-01
	C3	0.83388	3.75	4.39320e-01
	O1	-0.32059	2.9	5.85760e-01
	O2	-0.35127	3.00	7.11280e-01
	O3	-0.51740	2.96	8.78640e-01
	C4	0.47335	3.5	2.76144e-01
	F1	-0.16341	2.95	2.21752e-01
	F2	-0.16341	2.95	2.21752e-01
	F3	-0.16341	2.95	2.21752e-01

Table S2. Charge and van der Waals parameter for PF_6 anion

system	Atom	q [e]	σ [Å]	ε [kJ/mol]
PF_6^-	P	1.12	3.74	8.36800e-01
	F1	-0.32	3.1181	2.55224e-01
	F2	-0.32	3.1181	2.55224e-01
	F3	-0.32	3.1181	2.55224e-01
	F4	-0.32	3.1181	2.55224e-01
	F5	-0.32	3.1181	2.55224e-01
	F6	-0.32	3.1181	2.55224e-01

Table S3. Charge and van der Waals parameter for Li cation

System	Atom	q [e]	σ [Å]	ε [kJ/mol]
Li^+	Li	0.8	1.2599	2.61500e+01

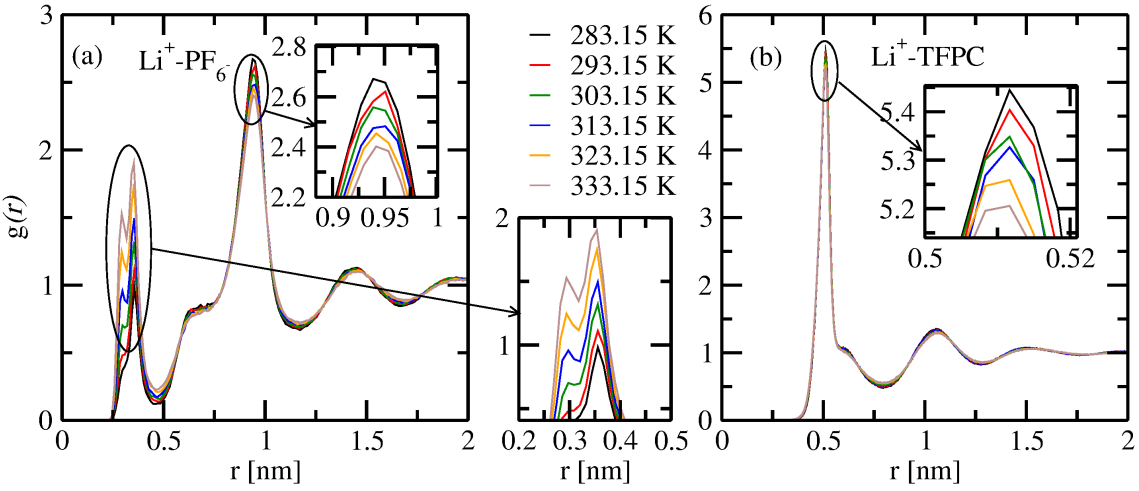

Figure S1. COM RDF of (a) Li^+-PF_6^-, and (b) Li^+-TFPC. Inset shows the zoomed view of the peaks.

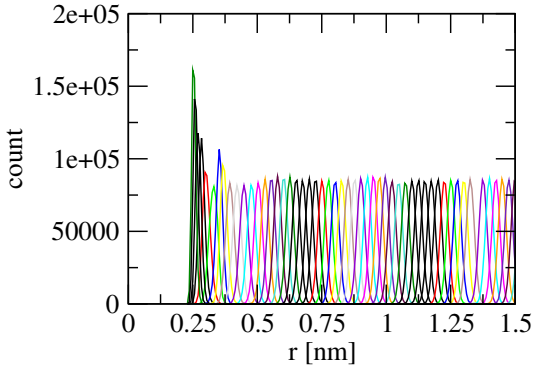

Figure S2. Histogram of showing the optimum overlap between the adjacent windows.