Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

X-Ray Absorption Spectroscopy of $LiBF_4$ in Propylene Carbonate: A Model Lithium Ion Battery Electrolyte

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Table S1: Comparison of large and small MD simulation box properties to previously published experimental findings of Takeuchi *et al.*[23]

	Large Box	Small Box	Experiment[23]
# PC in MD box	640	20	
# $LiBF_4$ in MD box	64	2	
Concentration (mol/L)	1.13	1.13	1.00
Concentration (mol/kg)	1.03	1.03	
Length of equilibration (ns)	3.2	6	
Length of the run (ns)	5.55	0.6	
Density (kg/m^3)	1257	1261	1251
D, solvent (1e-6 cm^2/s)	2.47118		2.2
D, anion (1e-6 cm^2/s)	1.06465		1.5
D, Li+ (1e-6 cm^2/s)	0.901052		0.9
Conductivity, no Finite Size Correction (mS/cm)	3.412459		3.6
Conductivity, hydro-corrected (mS/cm)	4.301659		3.6
dynamic degree of dissociation	0.41		0.4
fraction of free Li (r Li-B > 3.6 Å)	0.16	0.008	
fraction of free B (r Li-B > 3.6 Å)	0.06	0	