Lithium Salt Distribution and Thermodynamics in Electrolytes Based on Short Perfluoropolyether-*block*-Poly(ethylene oxide) Copolymers

Mahati Chintapalli, Ksenia Timachova, Kevin R. Olson, Sue J. Mecham, Joseph M. DeSimone, Nitash P. Balsara

In Figure S1a-c, WAXS profiles are shown for PFPE$_{E10}$-diol/LiTFSI electrolytes all salt concentrations, at 45 °C, 60 °C, and 75 °C, respectively. WAXS profiles at 30 °C and 90 °C are shown in Figure 1. The plots show that as salt concentration and temperature increase, scattering intensity decreases.
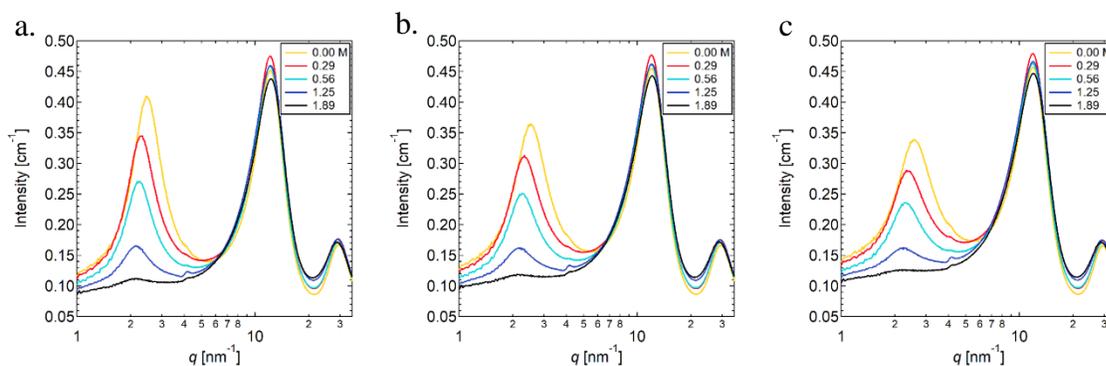

Figure S1. WAXS profiles are shown for PFPE$_{E10}$-diol/LiTFSI electrolytes at (a) 45 °C, (b) 60 °C, and (c) 75 °C. The color of each profile indicates the concentration of LiTFSI.

The solubility limits and salt concentrations used are reported in Table S1.[12,23]   Molar concentrations were calculated assuming that the molar volumes of the salt and polymer solvent are additive. The densities used in the calculation were 2.023 g cm^{-3} for LiTFSI, 1.77 g cm^{-3} for PFPE$_{D10}$-diol, and 1.73 g cm^{-3} for PFPE$_{E10}$-diol. The molar mass of LiTFSI is 287.09 g mol^{-1}.

Table S1.   Concentrations and solubility limits of electrolytes.   The solubility limits and concentrations are given below in mol L^{-1} (M), weight percent salt, and molar ratio of salt to polymer chains, n_{LiTFSI}.

	PFPE$_{D10}$-diol			PFPE$_{E10}$-diol		
	M	wt%	n_{LiTFSI}	M	wt%	n_{LiTFSI}
Solubility limit	0.67	11	.43	1.90	30	1.94
Concentration 1	0	0	0	0	0	0
Concentration 2	0.31	5	0.18	0.29	5	0.27
Concentration 3	0.57	9	0.35	0.56	9	0.52
Concentration 4	-	-	-	1.25	20	1.31
Concentration 5	-	-	-	1.89	30	2.23

In Figure S2, the values of the fit parameters a_0, a_1, and a_2 for the background function defined in equation 34 are given. The parameter a_0 represents diffuse background scattering phenomena, and a_1 and a_2 represent the width and height of the Lorentzian q_2 peak at approximately 10 nm^{-1}. The position of the peak, $q_{2,max}$ is a fixed parameter, given in Figure 2.
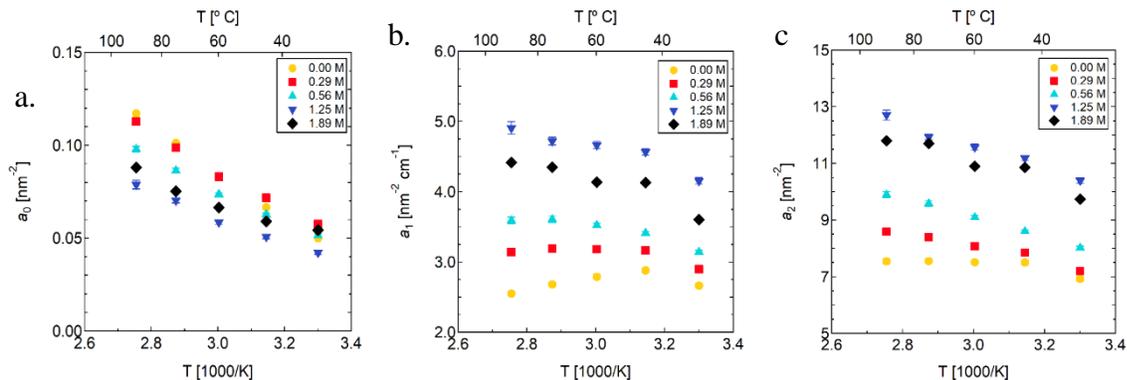

Figure S2. Background fit parameters, a_0, a_1, and a_2 are plotted in (a), (b), and (c), respectively, as functions of temperature, at different salt concentrations.

In Figure S3, fits of equation 35, $I_{dis}(q)$, to the background-subtracted data, $I_{data}(q) - I_{bg}(q)$ are shown for the temperatures between 30 and 90 °C, at various salt concentrations.
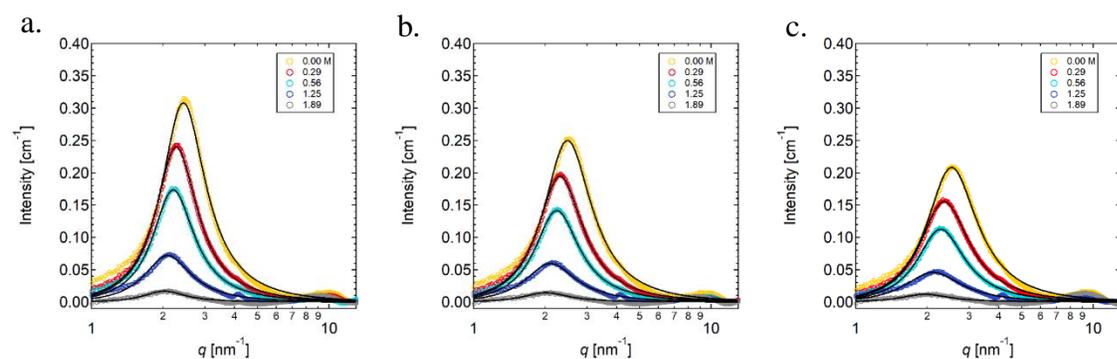

Figure S3. Fits of I_{dis} to background subtracted absolute scattering data, $I_{data} - I_{bg}$, at (a) 45 °C, (b) 60 °C, and (c) 75 °C.