Ion Transport Mechanisms in Lamellar Phases of Salt-Doped PS-PEO Block Copolymer Electrolytes: Supplementary Information

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I. UNITED ATOM PARAMETERS

Bonding Potential: $V_b = k_b(r - r_0)^2$		
Type	k_b $(kcal/mol/(\text{Å})^2)$	r_0 (Å)
CH_2-CH_2	250	1.54
CH-CH_2	250	1.54
CH-CH_3	250	1.51
CH(ring)-CH(ring)	250	1.40
C(ring)-CH(ring)	250	1.40
C(ring)-CH_2	250	1.51
O-CH	250	1.41
P-F	190	1.6

Angle Potential: $V_\theta = k_\theta(\theta - \theta_0)^2$		
Type	k_θ $(kcal/mol/rad^2)$	θ_0 (deg)
CH_2-CH_2-CH_2	120	114
CH(ring)-CH(ring)-CH(ring)	120	120
CH-CH_2-CH	62	114
C(ring) - CH(ring)-CH(ring)	120	120
CH(ring)- C(ring) -CH	120	120
CH_2- C(ring) - CH_2	120	120
CH_2-O -CH_2	60	114
CH_2-CH_2- O	50	112

Dihedral Potential: $V_\phi = \sum_{i=1}^{4} \frac{1}{2} k_{i\phi} \left(1 + (-1)^{(i+1)}\right) \cos(i\phi)$				
Type	$k_{1\phi}$ $(kcal/mol)$	$k_{2\phi}$	$k_{3\phi}$	$k_{4\phi}$
O-CH_2-CH_2-CH_2	0.7020	-0.2120	0.30600	0
CH_2-CH_2-O-CH_2	2.8828	-0.6508	2.2184	0
CH_2-CH_2-O-CH_3	2.8828	-0.6508	2.2184	0

CH_2-C(ring) -CH_2-C(ring)	1.4112	-0.2712	3.1452	0	
CH_3-C(ring) -CH_2-C(ring)	1.4112	-0.2712	3.1452	0	
Dihedral Potential: $V_\phi = \sum_{i=1}^{5} k_{i\phi} \cos(\phi)^{i-1}$					
Type	$k_{1\phi}$ $(kcal/mol)$	$k_{2\phi}$	$k_{3\phi}$	$k_{4\phi}$	$k_{5\phi}$
O-CH_2-CH_2-O	2	-6	1	8.4	2
Non-bonded Potential: $V_{ij} = 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \frac{q_i q_j}{r_{ij}}$; $\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$; $\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$					
Type	ϵ $(kcal/mol)$	σ (Å)	q (e)		
C(ring)	0.0596	3.700	0.0		
CH(ring)	0.1003	3.695	0.0		
CH	0.0199	4.650	0.0		
CH_2(PS)	0.0914	3.950	0.0		
CH_3	0.1947	3.750	0.0		
CH_2(PEO)	0.0914	3.950	0.25		
O	0.1093	2.800	-0.5		
Li	0.4000	1.400	1.0		
P	0.2000	3.742	0.7562		
F	0.0610	3.118	-0.2927		

TABLE S1: Interaction parameters for PS-PEO united atom model.

II. COUNTERION DIFFUSION

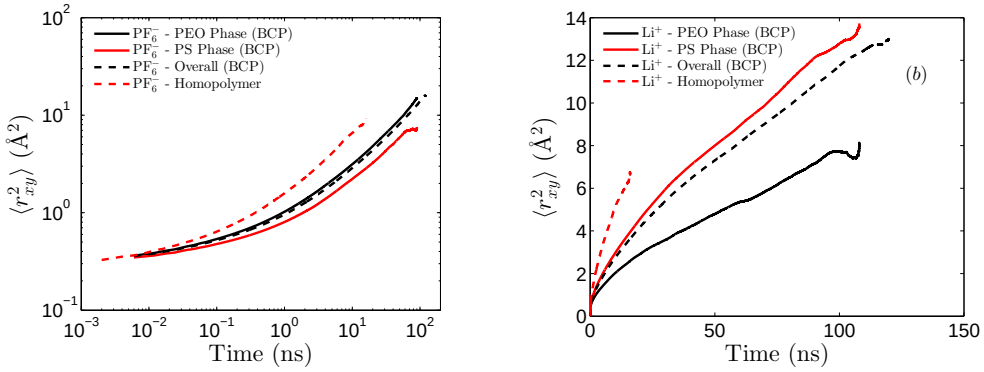

FIG. S1. (a) Counterion; (b) Ion diffusion comparison.

III. FIT TO RESIDENCE TIME AUTOCORRELATION FUNCTION

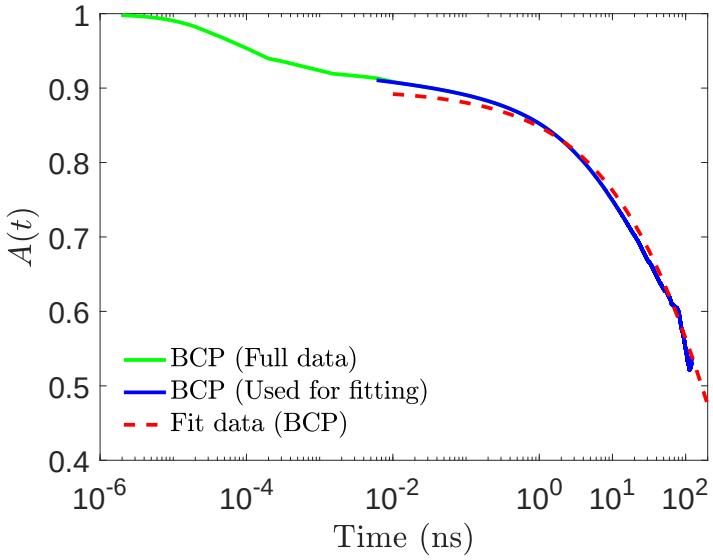

FIG. S2. Fit to Residence Time Correlation Function.

IV. ION HOPPING MECHANISM

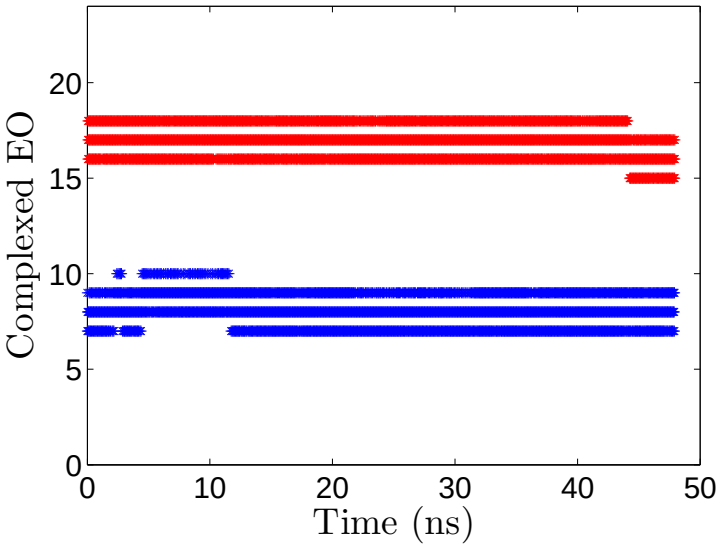

FIG. S3. Ion hopping mechanism with ions coordinated to two chains, but not hopping along any of the two chains.

V. REPRESENTATIVE C(N) PLOTS IN LOGARITHMIC SCALE

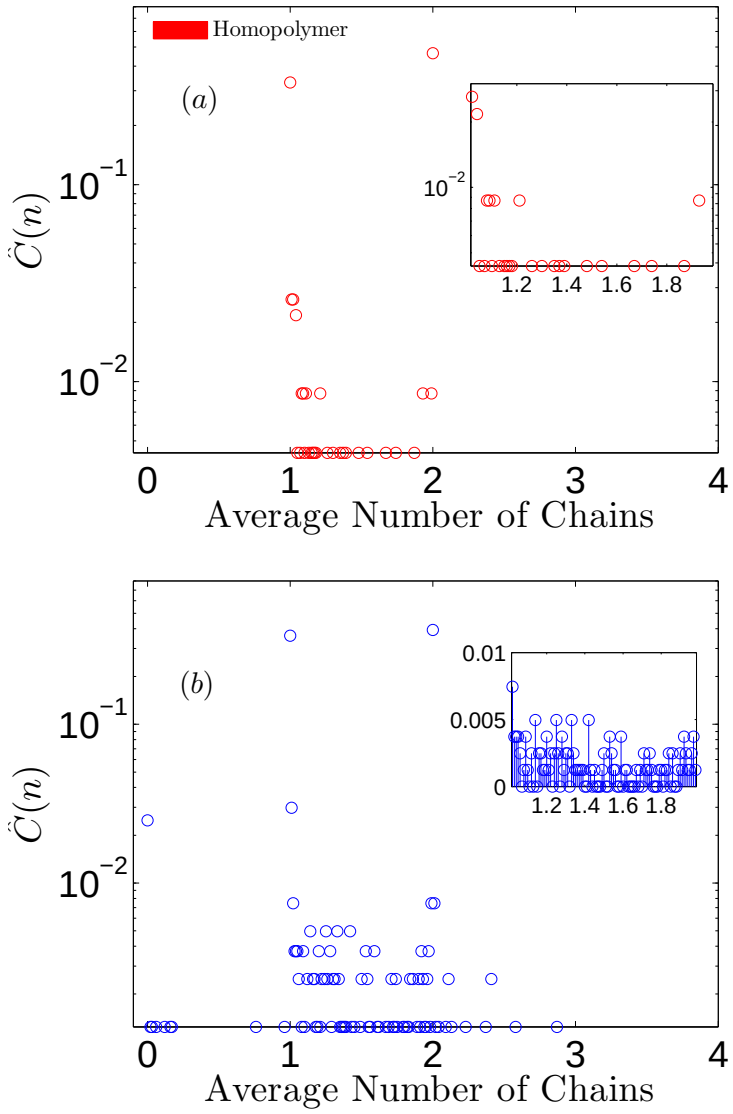

FIG. S4. Log plots for $C(n)$ for (a) homopolymer ; (b) BCP; at EO:Li=20:1.

VI. SALT EFFECTS ON RESIDENCE TIME AUTOCORRELATION FUNCTION

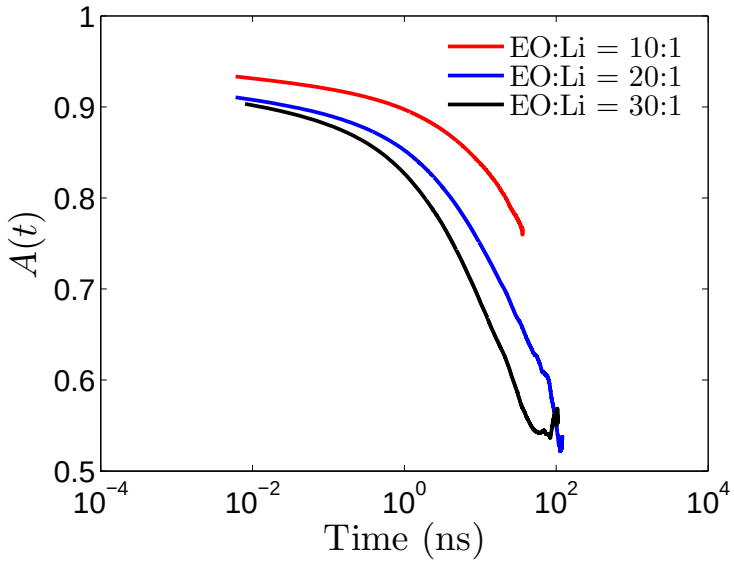

FIG. S5. Residence time autocorrelation function as a function of salt concentration. All residence times are fitted to the form: $A\exp\left(-\left(t/\tau\right)^{\beta}\right)$.