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Addition/Correction

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Correction to Multiscale Simulations of Lamellar PS−PEO Block Copolymers Doped with $LiPF_6$ Ions

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We recently reported (ref 1) a multiscale simulation study of the static properties of PS−PEO block copolymers doped with $LiPF_6$ salt. Unfortunately, while preparing the input file for homopolymer melt simulations, the coefficient and force-field OCCO dihedrals were switched with that of CCOC dihedrals. The input for block copolymers was correct, and hence the results and discussion pertaining to block copolymers (the main focus of the article) remain intact. However, the incorrect force-field parameters rendered some errors in the homopolymer results and impact comparisons to block copolymers. The new results (and the corresponding reference to old results) are discussed below:

1. The change in OCCO dihedral force-field parameter modifies some of the coordination results (ion−ion and ion−EO) discussed in Figures 7 and 8 of ref 1. Figure 7 of ref 1 (reproduced here in Figure 1 for reference) needs to be replaced with Figure 2 below. Although the quantitative values of the various coordination results in the homopolymer melt are changed, the qualitative trends remain identical to those shown in Figures 7a−c of ref 1. Hence, the discussion pertaining to Figures 7a−c (section 3.4.1 on pages 4547 and 4548 of ref 1) does not change.

To elaborate, the main focus of the discussion in section 3.4.1 of ref 1 was the influence of microphase segregation on the coordination strength of different ion/EO pairs. The main conclusions were that (i) the ion−ion and ion−EO coordination are enhanced in the PS domain of the BCP compared to the homopolymer melt and (ii) the ion−ion and ion−EO coordination in the PEO phase of the BCP melt were almost identical to those in the homopolymer melt. With the revised values of the OCCO dihedral parameters it can be seen (Figure 2) that the ion−ion and ion−EO coordination in PS phase in the BCP melt are enhanced compared to those in PEO phase of the BCP melt, demonstrating that the discussion remains unchanged for result (i) above. Similarly, the ion−ion and ion−EO coordination in the PEO phase of the BCP melt are almost identical to those in the homopolymer melt, suggesting that the discussion pertaining result (ii) also remain unchanged. However, the quantitative values, especially in the context of ion−ion coordination, *do* change, and the implications of such changes are discussed below.

2. Figure 8 of ref 1 (reproduced as Figure 3 below) is to be replaced by Figure 4 below. The results displayed in Figure 4 demonstrate that, irrespective of the salt concentration, the Li−PF_6 coordination remains the strongest in the PS phase. Such a result is consistent with the trends presented in ref 1.

The ratio of the first peaks in the Li−PF_6 coordination between the homopolymer melt and that in the PEO phase of the BCP melt is modified, especially at lower salt concentrations, from the results presented in ref 1. We found that at the lowest salt concentration investigated (EO:Li = 30:1) the peak height for Li−PF_6 coordination changed to 0.2 for the revised force fields as

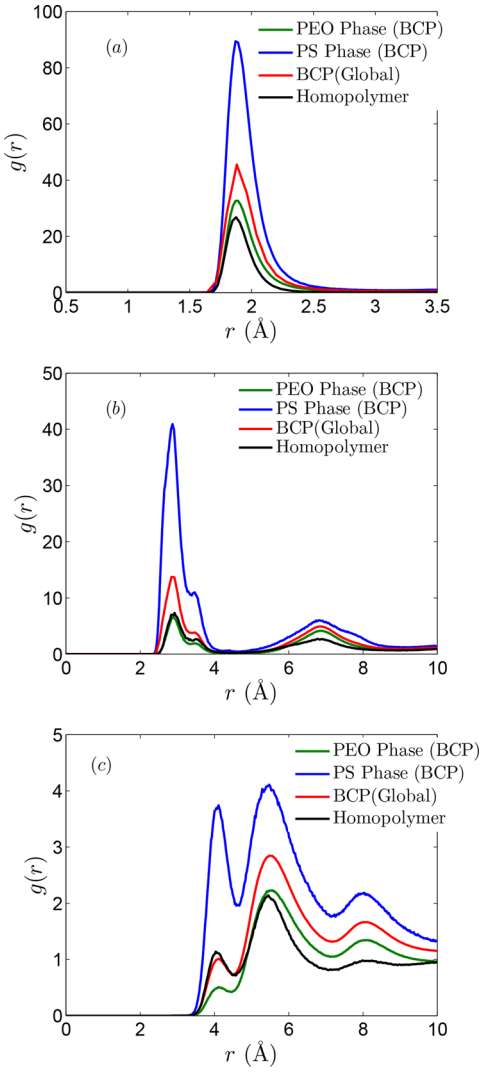

Figure 1. *Old* radial distribution functions for (a) Li−O, (b) Li−PF_6, and (c) P−O in PEO and PS domain separately. For comparison, the global averaged RDF in BCP and homopolymer are also shown.

opposed to a value of 16.0 in ref 1. Similarly, the peak heights changed from 12.0 to 2.0 and 9.0 to 4.0 for EO:Li = 20:1 and 10:1, respectively.

To explain the trends exhibited by the salt concentration dependence of the ratio of the peaks, we recall that in ref 1 the trends in Li−PF_6 coordination were rationalized as a combined consequence of the competing effects of (a) the stronger coordination between the ions in the PS melt and (b) the comparable

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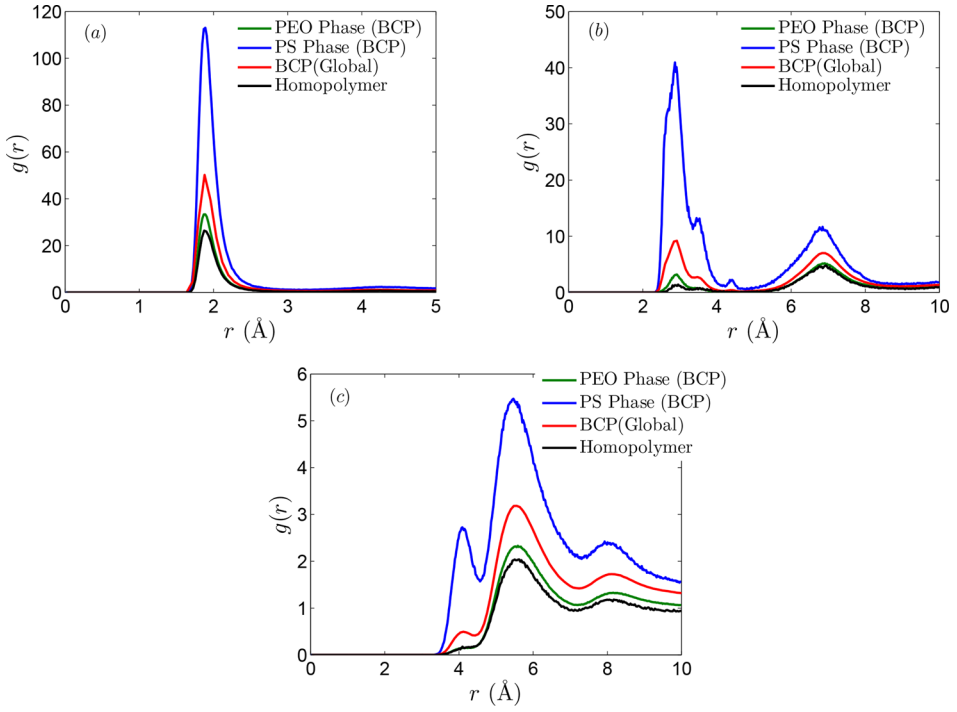

Figure 2. *Corrected* radial distribution functions for (a) Li−O, (b) Li−PF_6, and (c) P−O in PEO and PS domain separately. For comparison, the global averaged RDF in BCP and homopolymer are also shown.

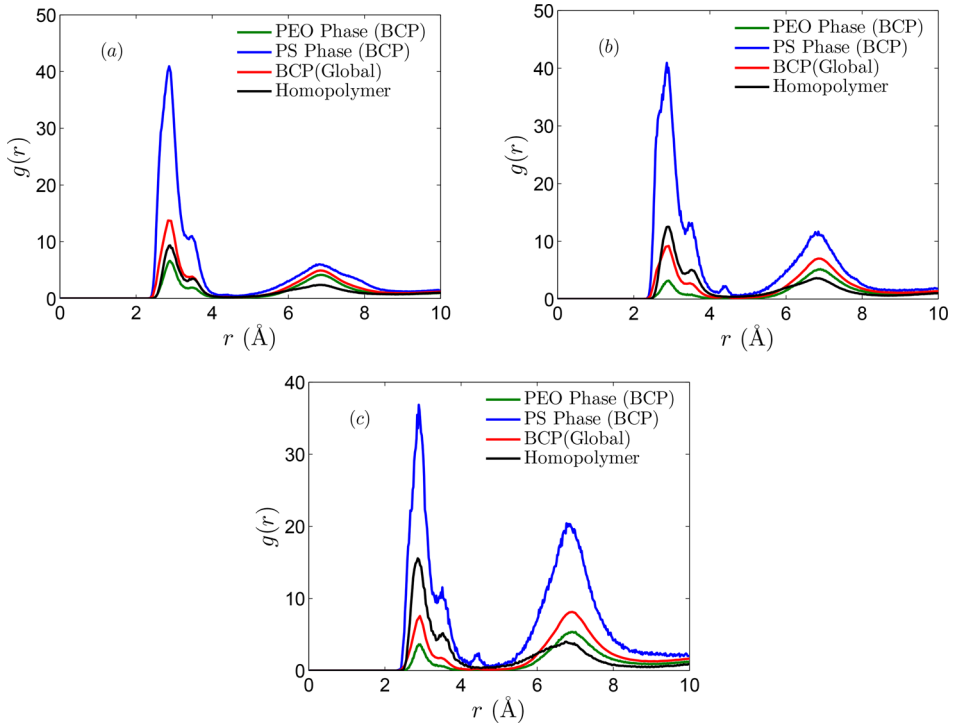

Figure 3. *Old* anion−cation RDFs as a function of salt concentration for EO:Li: (a) 10:1, (b) 20:1, and (c) 30:1.

or slightly weaker coordination between the ions in the PEO phase of the BCP melt compared to that in the pure homopolymer melt. With the revised results, we find that the coordination in the PEO phase of the BCP melt is stronger than that in the homopolymer melt (especially at low salt concentrations). As a consequence, the revised results manifest a more pronounced effect in the ratio of the peaks in Li−PF_6 coordination between the overall BCP melt and that pure homopolymer melt.

The new results for the Li−PF_6 coordination in homopolymers also render a modification to the statement in the abstract of ref 1. Explicitly, the statement "The cation−anion radial distribution functions (RDF) display stronger coordination in the block copolymer melts at high salt concentrations, whereas the trends are reversed for low salt concentrations." needs to be revised to "The cation−anion radial distribution functions (RDF) display stronger coordination in the block copolymer melts."

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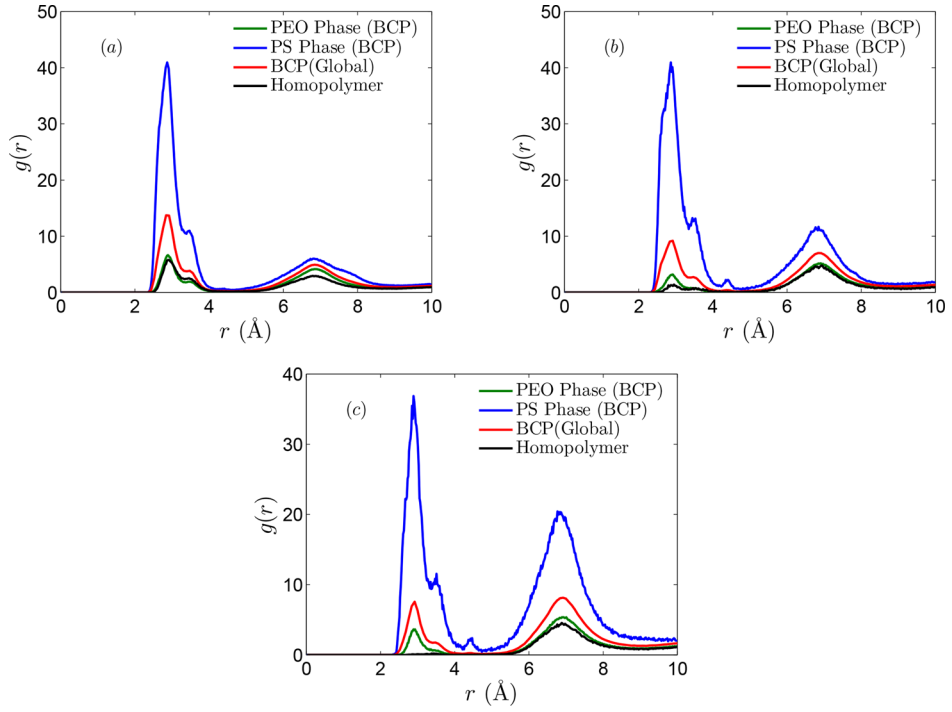

Figure 4. *Corrected* anion−cation RDFs as a function of salt concentration for EO:Li: (a) 10:1, (b) 20:1, and (c) 30:1.

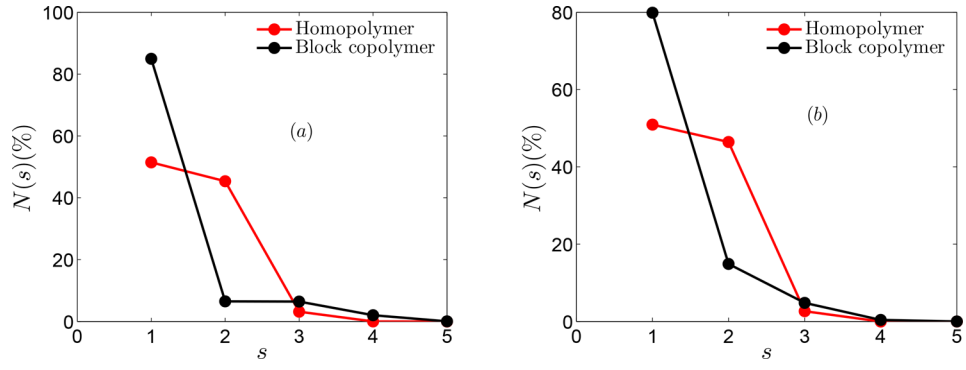

Figure 5. *Old* comparison of (a) $Li(PF_6)_{s-1}$ and (b) $Li_{s-1}PF_6$ clusters in block copolymers and homopolymers for EO:Li = 20:1.

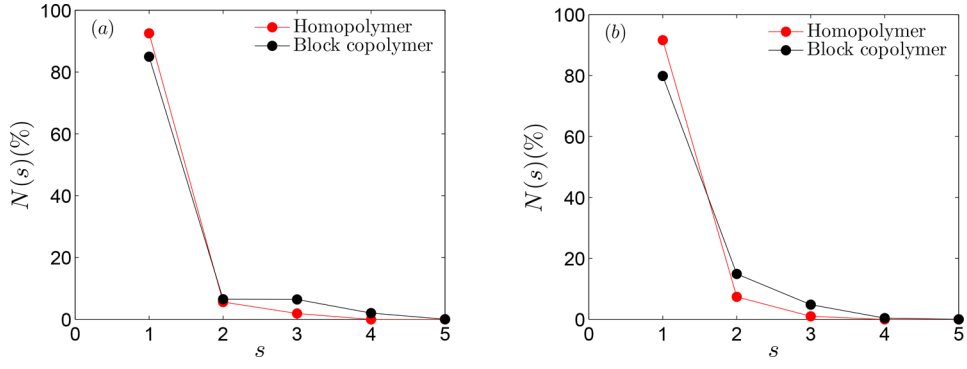

Figure 6. *Corrected* comparison of (a) $Li(PF_6)_{s-1}$ and (b) $Li_{s-1}PF_6$ clusters in block copolymers and homopolymers for EO:Li = 20:1.

3. Figures 13a and 13b of ref 1 (reproduced here in Figure 5) are to be replaced by Figures 6a and 6b, respectively, below. Figure 6a compares the $Li_{s-1}PF_6$ aggregates between block copolymer melt and homopolymer system for EO:Li = 20:1. Therein, it can be seen that the fraction of free Li^+ ions are higher in homopolymers compared to block copolymers. Our earlier results (Figure 13a) indicated a reverse trend, viz., that the fraction of free ions in BCPs to be higher. Similarly, the results of Figure 6b indicate that fraction of free ions in homopolymers is larger compared to BCP, a trend which is opposite to those displayed in Figure 13b of ref 1.

As a result of the above changes, the following sentence in section 3.6 (page 4552) of ref 1 is to be modified: "It can be seen

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that the fraction of free PF_6^- ions ($s = 1$) is larger in the case of block copolymers compared to that of the homopolymer. Correspondingly, a larger fraction of higher order pairs ($s > 1$) are seen in the case of homopolymers compared to that in the block copolymers" needs to be changed as "It can be seen that the fraction of free PF_6^- ions ($s = 1$) is larger in the case of homopolymers compared to that of the BCP. Correspondingly, a larger fraction of higher order pairs ($s > 1$) are seen in the case of BCP compared to that in the homopolymers." Finally, the sentence in the conclusion section "Further, the fraction of free ions was found to be smaller in the homopolymer compared to that of the block copolymer" is to be replaced with "Further, the fraction of free ions was found to be smaller in the block copolymer compared to that of the homopolymer."

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■ REFERENCES

(1) Sethuraman, V.; Mogurampelly, S.; Ganesan, V. *Macromolecules* **2017**, *50*, 4542.

■ NOTE ADDED AFTER ISSUE PUBLICATION

This paper was published on January 23, 2018, with an author's name misspelled. The error has been corrected and the revised version was republished on March 20, 2018.

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