Abstract Submitted
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Multiscale Simulations of PS-PEO Block Copolymers with LiPF$_6$ Ions in Lamellar Phase: Equilibrium Characteristics[1] VAIDYANATHAN SETHURAMAN, SANTOSH MOGURAMPALLY, VENKAT GANESAN, University of Texas at Austin — Multiscale simulations involving coarse-graining and inverse coarse-graining steps, are performed to characterize the structural equilibrium properties of polystyrene-polyethylene oxide (PS-PEO) block copolymer (BCP) melt in the ordered lamellar phase doped with Li-PF$_6$ salt. We compared the structural distribution functions between various entities in the system with that of PEO homopolymer melts. Anion-cation and cation-oxygen radial distribution functions show significantly stronger coordination in block copolymer melts when compared to the homopolymer melts. RDFs computed in PEO and PS domains separately show that the increased binding of the ion pairs in the BCP melts arise from the strong binding in the PS domains. Further, local structural distributions of cation-anion pairs reveal that the binding is stronger near the interface of the PS-PEO compared to that in the bulk of the PEO domain. The preceding quantities are also studied as a function of salt loading. An important result from such studies is that the number of free ions is found to decrease with increasing salt concentration in both block copolymer and homopolymer melts.

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Vaidyanathan Sethuraman
University of Texas at Austin

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