Abstract Submitted
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Multiscale Simulations of PS-PEO Block Copolymers with $LiPF_6$ Ions in Lamellar Phase: Dynamics[1] VAIDYANATHAN SETHURAMAN, SANTOSH MOGURAMPALLY, VENKAT GANESAN, University of Texas at Austin — Hybrid simulations, which include coarse-graining and inverse coarse-graining steps, are performed to characterize the dynamic properties of polystyrene-polyethylene oxide (PS-PEO) block copolymer (BCP) melt in the ordered lamellar phase doped with Li-PF_6 salt at the atomistic level. The ion dynamics in the block copolymer melts are studied as a function of salt concentration. Further, the ion dynamics are studied as a function of the distance from the interface to identify the spatial heterogeneity in ion dynamics. To identify the mechanism of ion transport, the inter- and intra- chain hopping are quantified.

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Vaidyanathan Sethuraman
University of Texas at Austin

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