

Abstract Submitted
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Hybrid Simulation Strategy for Simulating Self-Assembled Morphologies at the Atomistic Length Scales¹ VAIDYANATHAN SETHURAMAN, VENKAT GANESAN, Univ of Texas, Austin — In the context of Lithium-ion batteries, an enhancement in both ionic conductivity and mechanical properties, were observed for block copolymer electrolytes with increasing MW. On the contrary, when homopolymers were used as electrolytes, the ionic conductivity decreased with increasing MW. However, the origins of such increase in conductivity are unclear and are speculated to be tied to both the morphology and the atomistic details of the copolymer themselves. Motivated by such issues, we present a strategy to create ordered morphologies of block copolymers at the atomistic level using a combination of coarse-graining and inverse coarse-graining techniques. A mapping which is developed using the long-ranged structural mapping in the disordered phases will be utilized to generate self-assembled morphologies. In particular we focus on generating self-assembled morphologies of PS-PEO at the atomistic length scales. Statics and dynamics of such self-assembled morphologies will be presented and the effect of self assembly on the transport properties of ions will also be explored.

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