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Mechanisms Underlying Ionic Mobilities in Nanocomposite Polymer Electrolytes VENKAT GANESAN, BENJAMIN HANSON, VICTOR PRYAMITSYN, The University of Texas at Austin — Recently, a number of experiments have demonstrated that addition of ceramics with nanoscale dimensions can lead to substantial improvements in the low temperature conductivity of the polymeric materials. However, the origin of such behaviors, and more generally, the manner by which nanoscale fillers impact the ion mobilities remain unresolved. In this communication, we report the results of atomistic molecular dynamics simulations which used multibody polarizable force-fields to study lithium ion diffusivities in an amorphous poly(ethylene-oxide) (PEO) melt containing well-dispersed TiO_2 nanoparticles. We observed that the lithium ion diffusivities decrease with increased particle loading. Our analysis suggests that the ion mobilities are correlated to the nanoparticle-induced changes in the polymer segmental dynamics. Interestingly, the changes in polymer segmental dynamics were seen to be related to the nanoparticle's influence on the polymer conformational features. Overall, our results indicate that addition of nanoparticle fillers modify polymer conformations and the polymer segmental dynamics, and thereby influence the ion mobilities of polymer electrolytes.

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