

Abstract Submitted
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How to Improve Ion Transport in Polymer Nanocomposites? Insights from Atomistic Simulations SANTHOSH MOGURAMPALLY, VENKAT GANESAN, Univ of Texas, Austin — We present different strategies to enhance ion conducting properties of polymer nanocomposite electrolytes and their implications by varying the surface chemistries of the nanoparticles and interactions between nanoparticle and components of polymer-salt mixture. Our molecular dynamics simulations suggest that the ionic mobilities and conductivities correlate with the combined effects of the changes in polymer segmental dynamics and the modifications in the local environment of ionic species arising from the introduction of nanoparticles. In the presence of α , β and γ - Al_2O_3 nanoparticles, we observe a monotonic decrease of ionic conductivities and mobilities with the nanoparticle loading due to the corresponding slowing of polymer dynamics. However, with the introduction of the repulsive interactions between nanoparticle and components of polymer-salt mixture, we find an increase in the mobility and conductivity of the polymer nanocomposites. However, the repulsive interactions seem to decrease the elastic moduli in contrast to the moduli enhancing effects by attractive interactions.

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