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Molecular Dynamics Simulations of Ion Transport and Mechanisms in Polymer Nanocomposites[1] SANTOSH MOGURAMPELLY, VENKAT GANESAN, Department of Chemical Engineering, University of Texas at Austin, Austin, Texas 78712, United States — Using all atom molecular dynamics and trajectory-extending kinetic Monte Carlo simulations, we study the influence of Al_2O_3 nanoparticles on the transport properties of Li^+ ions in polymer electrolytes consisting of polyethylene oxide (PEO) melt solvated with $LiBF_4$ salt. We observe that the nanoparticles have a strong influence on polymer segmental dynamics which in turn correlates with the mobility of Li^+ ions. Explicitly, polymer segmental relaxation times and Li^+ ion residence times around polymer were found to increase with the addition of nanoparticles. We also observe that increasing short range repulsive interactions between nanoparticles and polymer membrane leads to increasing polymer dynamics and ion mobility. Overall, our simulation results suggest that nanoparticle induced changes in conformational and dynamic properties of the polymer influences the ion mobilities in polymer electrolytes and suggests possible directions for using such findings to improve the polymer matrix conductivity.

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