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Ion Transport via Structural Relaxations in Polymerized Ionic Liquids VENKAT GANESAN, Univ of Texas, Austin, SANTOSH MOGURAMPALLY, Institute for Computational Molecular Science, Temple University — We study the mechanisms underlying ion transport in poly(1-butyl-3-vinylimidazolium-hexafluorophosphate) polymer electrolytes. We consider polymer electrolytes of varying polymerized ionic liquid to ionic liquid (polyIL:IL) ratios and use atomistic molecular dynamics (MD) simulations to probe the dynamical and structural characteristics of the electrolyte. Our results reveal that anion diffusion along polymer backbone occurs primarily *via* the formation and breaking of ion-pairs involving *three* polymerized cationic monomers of *two* different polymer chains. Moreover, we observe that the ionic diffusivities exhibit a direct correlation with the structural relaxation times of the ion-pairs and hydrogen bonds (H-bonds). These results provide new insights into the mechanisms underlying ion transport in polymerized ionic liquid electrolytes.

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