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Mechanism of Ion Diffusion in Coarse-Grained Ionomer Melts
LISA M. HALL, The Ohio State University, MARK J. STEVENS, AMALIE L. FRISCHKNECHT, Sandia National Laboratories — Ionomers (polymers with a small amount of charged groups) have been identified as possible single ion conducting battery electrolytes. A barrier their use in such applications is that the strong electrostatic interactions lead to ionic aggregation and can make ion diffusion very slow. In order to understand the physics underlying ionomer dynamics and especially how charge transport occurs, we perform molecular dynamics simulations. Our model has polymers with charged groups either in the backbone or pendant to it, explicit counterions, and long-range Coulomb interactions. Depending on placement, amount, and spacing of the ionic groups, various morphologies of ionic aggregates are formed. We find for all systems, ions can rearrange locally within the ionic aggregates on a relatively short timescale. Ions can move a longer distance when they rearrange collectively on a longer timescale, that is especially long for systems with discrete ionic aggregates. Because of this, a typical ion trajectory shows mostly small movements and rare large, sudden movements. However, these features are not due to 'hopping' as typically understood. Instead, nearby aggregates of ions join together, rearrange, and later break apart, during which time some ions are exchanged and appear to have 'hopped'.

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