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Coarse-Grained Simulation of Ion Diffusion in Polymer Melts: Effect of Physical Crosslinking and Finite Concentration ZHEN-GANG WANG, UMI YAMAMOTO, California Institute of Technology — We present a coarse-grained simulation framework to study long-time dynamics of lithium ions in unentangled polymer melts. Effects of strong cation-monomer binding are modelled by formation of reversible bonds, and monomer-specific binding features enter via bond lifetime and coordination number, which can be estimated from atomistic simulations. Two competing mechanisms control the cation transport: successive replacement of dynamic bonds, and motion of the "branched" polymer cluster formed by a cation. Either channel can dominate the long-time diffusion depending on chain lengths and/or the bond lifetime relative to the Rouse time. At high concentrations, cations crosslink the polymers into a transient network, which significantly slows down the relaxation of the polymers, resulting in the non-monotonic dependence of ion conductivity on concentration, in qualitative agreement with experiment.

Zhen-Gang Wang
California Institute of Technology

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