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**Ion Dynamics in Model Ionomer Melts as a Function of Polymer Architecture** LISA M. HALL, MARK J. STEVENS, AMALIE L. FRISCHKNECHT, Sandia National Laboratories — Ionomers, polymers with a small fraction of covalently bound ionic groups, have potential advantages as solid, single ion conducting electrolytes in future batteries. However, the strong electrostatic interactions in these materials can make counterion diffusion unacceptably slow. Understanding how controllable molecular properties affect ionomer dynamics could spur design of improved materials. With this goal, we perform molecular dynamics simulations of ionomers of various architectures and evaluate their dynamic behavior. Our model of coarse-grained polymers with explicit counterions captures the fundamental physics while allowing access to the long time and length scales relevant to ionomer melts. The simulated structure factors reproduce the trends found in experimental scattering of recently synthesized ionomers with controlled precise or pseudorandom spacing of charged groups along the chain. We calculate counterion diffusion constants and other dynamic properties, which can change significantly depending on the location and spacing of charges along the chain. Randomly spaced materials can have slower or faster dynamics than periodically spaced materials, depending on whether the sequence is completely random or pseudorandom, which will be discussed.

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