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Molecular dynamics simulations of ionic aggregates in a coarse-grained ionomer melt[1] LISA HALL, MARK STEVENS, AMALIE FRISCHKNECHT, Sandia National Laboratories — Ionomers (polymers with a small fraction of covalently bound ionic groups) have potential application as solid battery electrolytes. Understanding ion transport is essential for such applications. A key question is how molecular properties affect ionic aggregation and counterion dynamics. Recent experimental advances allowed synthesis and extensive characterization of ionomers with a precise spacing of charged groups, which is ideal for comparison with simulations. We use coarse-grained molecular dynamics to simulate ionomers with charged beads placed periodically either in the polymer backbone or pendant to the backbone. The polymers, along with counterions, are simulated at melt densities. Pendant ions at low dielectric form roughly spherical aggregates with liquidlike interaggregate order, qualitatively different from the aggregate morphology of analogous linear ionomers. The effects of dielectric constant and backbone spacing of charged beads on ionic structure and diffusion will be discussed.

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