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Dynamics and morphologies of course-grained ionomer melts under an external electric field CHRISTINA TING, MARK STEVENS, AMALIE FRISCHKNECHT, Sandia Natl Labs — Ionomers have been identified as potential solid electrolytes in battery applications. However, these systems are hindered by strong electrostatic interactions that can lead to ionic aggregation, making ion diffusion very slow. To develop a molecular understanding of how the ion transport depends on the system morphology and ultimately the ionomer chemistry, we perform molecular dynamics simulations. We apply an external electric field to a melt of course-grained polymers with charged groups along or pendant to the backbone, and explicit counterions. We observe ionic aggregate morphologies that merge and whose shape anisotropy, depending on the strength of the field, may decrease or increase (along the field direction). We also quantify the dependence of the drift mobility of the ions on the aggregate morphologies and the field strength.

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