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Nonequilibrium Simulations of Ion Dynamics in Ionomer Melts

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Ionomers, polymers containing a small fraction of covalently bound ionic groups, are of interest as possible electrolytes in batteries. However, to date ionomers do not have sufficiently high conductivities for practical application, most likely because the ions tend to form aggregates, leading to slow ion transport. To build a better understanding of the relationships among ionomer chemistry, morphology, and ion transport, we have performed a series of molecular dynamics simulations and connected aspects of these simulations with experiment. In previous work using both atomistic and coarse-grained models, we showed that precise ionomers (with a fixed spacing between ionic groups along the polymer backbone) exhibit a range of ionic aggregate morphologies, from discrete clusters to percolated aggregates. In this talk I will describe recent simulations of our coarse-grained ionomer melts in an applied electric field. From a constant applied field, we are able to extract the ion mobilities and hence conductivities. We find that ionomers with percolated ionic aggregate morphologies have higher ion mobilities and hence higher conductivities. Application of an oscillating electric field enables us to calculate the frequency-dependent conductivity of the model ionomer melts. The real part of the conductivity has a high frequency peak associated with plasma oscillations, and a very broad low frequency peak associated with ion motions in ionic aggregates. I will end with comments on the connections to atomistic simulations and to experimental probes of ion dynamics.

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