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Atomistic Simulations Reveal a Surprising Variety of Morphologies in Precise Ionomers MARK STEVENS, DAN BOLINTINEANU, AMALIE FRISCHKNECHT, Sandia National Labs — Ionomers are being investigated as potential solid electrolytes in battery applications, due to their unique electrical properties. However, the relationships between ionomer chemistry, morphology and ion transport are poorly understood, which has hindered the development of ionomer-based batteries. To this end, we report atomistic molecular dynamics (MD) simulations of a model ionomer (polyethylene-co-acrylic acid) neutralized with different ions at various neutralization levels. The structure factor computed from the simulations is in good agreement with experimental X-ray scattering data. The simulations provide new insight into the shape, size and composition of ionic aggregates. In particular, we observe a wide variety of aggregate morphologies, ranging from small spherical aggregates to string-like shapes and large percolated networks. The unexpected morphologies of these ionic aggregates imply the need for a new interpretation of scattering spectra for these materials. We quantify cation-anion and oxygen-hydrogen association, the two interactions primarily responsible for aggregate formation, and report detailed information pertaining to local structures around cations, which is difficult to obtain experimentally and may have important consequences for ion transport.

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