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Morphology and Aggregate Local Structure of Precise Polyolefins with Associating Pendant Groups FRANCISCO BUITRAGO, University of Pennsylvania, DAN BOLINTINEANU, MARK STEVENS, AMALIE FRISCHKNECHT, Sandia National Laboratories, KAREN WINEY, University of Pennsylvania, WINEY GROUP TEAM, FRISCHKNECHT/STEVENS GROUP TEAM — Polyolefins containing acid and/or ionic pendant groups have specific interactions that produce complex and hierarchical morphologies providing a remarkable set of properties. Despite the widespread industrial use of such materials, rigorous morphology-property relationships remain elusive due to structural heterogeneities in the available copolymers. Recently, linear polyethylenes with associating pendant groups separated by a precisely controlled number of carbon atoms have been synthesized by acyclic diene metathesis (ADMET) polymerization. At room temperature, X-ray scattering shows that the molecular uniformity of these materials results in periodic morphologies of the microphase separated ionic groups. Above their transition temperatures (T_g, T_m), loss of the periodic structures occurs due to polyethylene crystals melting. The morphologies of precise ionomers at elevated temperatures were further investigated via atomistic molecular dynamics (MD) simulations. The simulations complement the X-ray scattering experiments by providing a clear picture of the aggregate shape and size as a function of counterion type, neutralization level and spacer length.

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