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Effect of Carboxyl Groups on Ionomer Properties from Molecular Dynamics Simulations[1] JANANI SAMPATH, LISA M. HALL, Ohio State Univ - Columbus — Ionomers are polymers with a small fraction of charged groups covalently bound to the non-polar polymer backbone, used in packaging and other applications. We consider ionomers and counterions with no solvent, in which the aggregation of ions significantly impacts overall material properties. Prior work established a useful coarse-grained model for fully neutralized acetic acid based ionomers, which include COO^- and Na^+ but no COOH groups. To better model typical experimental systems that are only partially neutralized, we use additional "sticker" groups that represent COOH. These stickers are similar to uncharged monomers but with adjusted Lennard-Jones interaction strengths with each other and with ionic groups. Sticker-sticker interactions are radially symmetric (in contrast to true hydrogen bonding), however, aggregate morphologies obtained using the sticker-based model are in good agreement with prior atomistic simulation results. We analyze the structure (including scattering profiles) and dynamics of partially neutralized ionomers with differing chain architectures. Rheological properties such as viscosity and stress relaxation obtained from equilibrium stress fluctuations will also be discussed.

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