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**Brownian Dynamics Studies of Morphology and Dynamics of Associative Ionomers**[1] ANIKET BHATTACHARYA, University of Central Florida, MONOJOY GOSWAMI, SANAT K. KUMAR, Rensselaer Polytechnic Institute — We propose to utilize computer simulations to understand the morphology and the viscoelastic properties of melts of polymers which have charges on their backbone with small counterions being carried along for charge neutrality ("ionomers"). While there has been significant theoretical and experimental research performed on ionomers, little systematic simulation work has been conducted which explicitly incorporates the long range Coulomb interaction among the charges on the polymer backbone and the counterions. We shall utilize Molecular dynamics simulations to study the aggregation behavior and reversible gelation of these materials, particularly focusing on the molecular aspects which drive the formation of local clusters studied recently by transmission electron microscopy (STEM)[†]. We will also study the unusual viscoelastic response, shear induced morphologies, and melting of the Coulomb gel using non-equilibrium molecular dynamics (NEMD) simulations.
[†]B. Kirkmeyer, A, Taubert, J-S Kim, K. I. Winey, Macromolecules **35**, 2648 (2002).

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