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Morphology and Dynamics of Ion Containing Polymers using Coarse Grain Molecular Dynamics Simulation MONOJOY GOSWAMI, BOBBY SUMPTER, Oak Ridge National Laboratory — Ion containing polymers are of particular interest in polymer batteries and membranes for separation chemistry applications. With the increasing interest in this field, novel and modern experimental techniques have been developed to design better materials, however, the fundamental understanding of these polymers, their morphology and ion/counterion dynamics are still not very well understood. We present a coarse grain simulation study to understand the structural detail and physics of ion/counterion dynamics. We do implicit as well as explicit solvent calculation to observe the effect of dielectric constant and temperature on dynamics of polymer chain and ion/counterion. The results are then compared with the small angle neutron scattering experiments. These works will help design better materials for future applications.

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