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Electrostatic effects on clustering and ion dynamics in ionomer melts BORAN MA, TRUNG NGUYEN, VICTOR PRYAMITSYN, MONICA OLVERA DE LA CRUZ, Northwestern University — An understanding of the relationships between ionomer chain morphology, dynamics and counter-ion mobility is a key factor in the design of ion conducting membranes for battery applications. In this study, we investigate the influence of electrostatic coupling between randomly charged copolymers (ionomers) and counter ions on the structural and dynamic features of a model system of ionomer melts. Using coarse-grained molecular dynamics (CGMD) simulations, we found that variations in electrostatic coupling strength (Γ) remarkably affect the formation of ion-counter ion clusters, ion mobility, and polymer dynamics for a range of charged monomer fractions. Specifically, an increase in Γ leads to larger ionic cluster sizes and reduced polymer and ion mobility. Analysis of the distribution of the radius of gyration of the clusters further reveals that the fractal dimension of the ion clusters is nearly independent from Γ for all the cases studied. Finally, at sufficiently high values of Γ, we observed arrested heterogeneous ions mobility, which is correlated with an increase in ion cluster size. These findings provide insight into the role of electrostatics in governing the nanostructures formed by ionomers.

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