

Abstract Submitted
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Correlation between superionic behavior and ion aggregation in PEO-based single-ion conductors¹ KAN-JU LIN, JANNA MARANAS, Pennsylvania State University — PEO-based ionomers as solid polymer electrolytes offer the advantage of preventing reverse polarization in batteries by covalently bonding the anion to the PEO backbone. These ionomers form ion aggregates, which reduces the polymer mobility. Since ion transport is coupled to polymer dynamics, these systems have low conductivity. We therefore need a mechanism that decouples ion conduction and PEO dynamics to improve conductivity. We investigate these conduction mechanisms using different models in MD simulations of PEO based benzene sulfonate ionomers. The study shows that these ionomers are capable of showing superionic behavior. The geometry of benzene rings helps aligning the anions, assisting in the formation of chain-like aggregates. The simulations show that the chain-like aggregates result in ionomer conductivity greater than its self-diffusion limits. The superionic behavior is attributed to a charge transfer between two chain ends (conduction sites): a cation hopping to one chain end and the cation at the other end hopping to a nearby site. This allows long range positive charge transfer while the cations only move locally. The results suggest that the superionic behavior depends on the length and lifetime of the chain aggregates. While a long chain reduces the overall number of conduction sites, a short chain prevents long range charge transfer. If the lifetime of an aggregate is shorter than the hopping time for cations, the hopping will not occur and the self-diffusion dominates conductivity.

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