



~~~~ Polymer Physics Seminar ~~~~

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301 Steidle Bldg.

A Molecular Look at PEO-Based Ionomers for Battery Application

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. The practical limitation is that the ionomer conductivity is insufficient to power a device. The cations in these ionomers occupy a wide range of coordination states. We use molecular dynamics simulations of PEO based benzene sulfonate ionomers to study the correlation between cation coordination states and their mobility. We further investigate the effect of binding the anion to the PEO backbone by comparing these ionomers to the PEO-salt counterparts. The simulations show that the geometry of the benzene ring helps align the anions, assisting in the formation of chain-like aggregates. These aggregates crosslink different backbone segments and therefore reduce PEO 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. The simulations show that these ionomers are capable of showing superionic behavior, in which the conductivity is greater than the ions' 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 anion at the other end hopping to a nearby site. This allows long range positive charge transfer while the anions only move locally. The superionic behavior depends on the lifetime and the length of the chain-like aggregates, and will be discussed in the presentation.