

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Controlling ion aggregation and conduction in PEO-based ionomers.** DAVID CALDWELL II, JANNA MARANAS, Pennsylvania State Univ — PEO-based ionomers are ideal for reducing concentration polarization found in typical solid polymer electrolytes. This is achieved by binding the anion to the polymer backbone, significantly reducing the anions mobility. Ion aggregation is prevalent in these systems, but their influence on SPE performance is difficult to study experimentally. We present results of molecular dynamics simulations that explore the relationship between ion content and temperature on ion aggregation, polymer motion, and ion conduction. An unforeseen result of ionomers is the creation of string like aggregates that form conduction pathways in the amorphous region. These conduction pathways allow for a partial decoupling of ion conduction with polymer dynamics. The improvement in conductivity through the use of ion aggregates can be quantified by calculating the inverse of the Haven Ratio, dubbed f-value. Typical SPEs have an f-value less than 0.2, while the ionomers of study exhibit f-values near unity or higher. Understanding what properties influence the development and use of these conduction pathways will provide insight for further development of solid polymer electrolytes.

David Caldwell II  
Pennsylvania State Univ

Date submitted: 14 Nov 2014

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