Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

The interplay of ion crosslinking, free ion content, and polymer mobility in PEO-based single-ion conductors KAN-JU LIN, JANNA MARANAS, The Pennsylvania State University — We use molecular dynamics simulation to study ion clustering and dynamics in ion containing polymers. This PEO based single-ion conducting ionomer serves as a model system for understanding cation transport in solid state polymer electrolytes (SPEs). Although small-angle x-ray scattering does not show an ionomer peak, we observer various cation-anion complexes in the simulation, suggesting ionomer backbones are crosslinked through ion complexes. These crosslinks reduce the adjacent PEO mobility resulting in a symmetric mobility gradient along the PEO chain. We vary the cation-anion interaction in the simulation to observe the interplay of cation-anion association, polymer mobility and cation motion. Cation-anion association controls the number of free ions, which is important in ionic conductivity when these materials are used as SPEs. Polymer mobility controls how fast the free ions are able to move through the SPE. High conductivity requires both a high free ion content and fast polymer motion. To understand the connection between the two, we "tune" the force field in order to manipulate the free ion content and observe the influence on PEO dynamics.

Kan-Ju Lin
The Pennsylvania State University

Date submitted: 09 Dec 2009 Electronic form version 1.4