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Correlation between cation conduction and ionic morphology in a PEO-based single ion conductor KAN-JU LIN, JANNA MARANAS, Pennsylvania State University — We use molecular dynamics simulation to study ion transport and backbone mobility of a PEO-based single ion conductor. Ion mobility depends on the chemical structure and the local environment of the ions, which consequently impact ionic conductivity. We characterize the aggregation state of the ions, and assess the role of ion complexes in ionomer dynamics. In addition to solvated cations and pairs, higher order ion clusters are found. Most of the ion clusters are in string-like structure and cross-link two or more different ionomer chains through ionic binding. Ionic crosslinks decrease mobility at the ionic co-monomer; hence the mobility of the adjacent PEO segment is influenced. Na ions show slow mobility when they are inside large clusters. The hopping timescale for Na varies from 20 ns to 200. A correlation is found between Na mobility and the number of hops from one coordination site to another. Besides ether oxygens, Na ions in the ionomer also use the anion and the edge of the cluster as hopping sites. The string-like structure of clusters provide less stable sites at the two ends thus ions are more mobile in those regions. We observed Grotthus like mechanism in our ionomer, in which the positive charge migrates within the string-like cluster without the cations actually moving.

Kan-Ju Lin
Pennsylvania State University

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