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**Exploring Li+ Potential Energy Surface in Poly(ethylene oxide)-based Sulfonate Ionomers**[1] HUAI-SUEN SHIAU, MICHAEL J. JANIK, RALPH H. COLBY, Pennsylvania State University, University Park — Ion-containing polymers are of interest as single-ion conductors for use as electrolytes in electrochemical devices, including lithium ion batteries. Current ion conductivities of the best ionomers are roughly 100X too small for practical applications and have a small fraction of their Li+ counterions participating in conduction. We are using ab initio methods to investigate the Li+ conduction mechanism, and specifically the role of transient positive triple ions (Li+A-Li+) in the conduction process. The positive triple ion has a lower energy separated state that allows for facile transport, if there is a pair within 1.4 nm. We will discuss the competition between cation solvation with ether oxygen atoms and cation-anion interaction. The importance of anion-anion separation in altering Li+ hopping barriers will be examined, as well as the variation in hopping rates with solvent identity. Ab initio calculations are used to evaluate the relative energy of ion states (contact and separated states), and this analysis is used to explain experimental phenomena of Li+ mobility in ionomers.

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