

Abstract Submitted  
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**Ion Correlation and Transport in Polymer Electrolytes at Finite Salt Concentrations; Coarse-Grained Simulation Study** UMI YAMAMOTO, ZHEN-GANG WANG, California Institute of Technology — We present results from coarse-grained simulation for ion dynamics and structures in dry polymer electrolytes. To capture the thermodynamic, kinetic, and system-specific aspects of ion solvation and clustering, cation-monomer complexation is modeled via functionalized physical bonds whose functionality and lifetime vary due to local availability of binding monomers and competition with Coulombic interaction. By varying salt concentration, cation-monomer binding energy, dielectric constant, and maximal functionality of the physical bonds, we systematically study the growth of ion clustering activity as characterized by packing structures, and associated changes in electric conductivity via single-ion and collective charge mobility. Deviations from Nernst-Einstein predictions, and comparisons with existing experiments for concentration dependence of conductivity will be discussed.

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