

Abstract Submitted
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Concentration Dependence of Ionic Correlation and Its Relation to Non-Ideality UMI YAMAMOTO, ZHEN-GANG WANG, Caltech — For salt-doped polymer electrolytes, a number of spectroscopic studies report that anions are more likely to be in contact with cations as salt concentration increases, implying that the ionic conductivity exhibits greater non-ideality, namely, growing deviation from Nernst-Einstein relation, due to the increased number of spatially-close ion pairs. However, the validity of this expectation remains unclear since the spectroscopic (structural) and the conductivity (dynamical) measurement resolve different time-scales, obscuring the fundamental relationship between the ion pairing and the non-ideal conductivity. In this work, we investigate the above question based on equilibrium and non-equilibrium coarse-grained simulations for model polymer electrolytes. By quantifying the structural and dynamical correlation of ions in a distinctive statistical-mechanical manner, and comparing them with the concentration dependence of the non-ideality, we aim to provide microscopic insights about how the natures of the two correlations differ, and how they affect the conductivity as a function of concentration. Their relative significance compared to the concentration dependence of the matrix viscosity is also discussed.

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