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Ion Transport and Structural Properties of Polymeric Electrolytes and Ionic Liquids from Molecular Dynamics Simulations¹

OLEG BORODIN, University of Utah, Wasatch Molecular Inc.

Molecular dynamics simulations are well suited for exploring electrolyte structure and ion transport mechanisms on the nanometer length scale and the nanosecond time scales. In this presentation we will describe how MD simulations assist in answering fundamental questions about the lithium transport mechanisms in polymeric electrolytes and ionic liquids. In particular, in the first part of the presentation the extent of ion aggregation, the structure of ion aggregates and the lithium cation diffusion in binary polymeric electrolytes will be compared with that of single-ion conducting polymers. In the second part of the talk, the lithium transport in polymeric electrolytes will be compared with that of three ionic liquids ([emim][FSI] doped with LiFSI , [pyr13][FSI] doped with LiFSI, [emim][BF₄] doped with LiBF₄). The relation between ionic liquid self-diffusion, conductivity and thermodynamic properties will be discussed in details. A number of correlations between heat of vaporization H_{vap} , cation-anion binding energy ($E_{+/-}$), molar volume (V_m), self-diffusion coefficient (D) and ionic conductivity for 29 ionic liquids have been investigated using MD simulations. A significant correlation between D and H_{vap} has been found, while best correlation was found for $-\log((D V_m))$ vs. $H_{vap}+0.28E_{+/-}$. A combination of enthalpy of vaporization and a fraction of the cation-anion binding energy was suggested as a measure of the effective cohesive energy for ionic liquids.

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