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Correlating Solution Structure to Electrolyte Properties

Wednesday, September 11, 2013
2:15 p.m.
101 Goergen Hall

The development of advanced battery technologies is a crucial need for the electrification of vehicles and widespread adoption of renewable energy sources such as wind and solar energy. Many battery technologies are limited, however, by the electrolyte formulations used (i.e., the solvent-salt mixtures which conduct ions for the battery reactions). The electrolyte's properties are often the key determinants for the battery's usable energy and power, operating temperature range, lifetime/durability, safety, cost, etc.

Deconvoluting the myriad factors which govern electrolyte properties is possible by examining in detail the link between molecular-level interactions and electrolyte solution structure. Understanding solution structure, however, remains one of the great challenges of science. A synergistic experimental approach has been employed involving: phase diagrams/solvate crystal structures, vibrational spectroscopic characterization of ion solvation/ionic association interactions and physicochemical/electrochemical property measurements. This work clearly delineates which solvent and anion structural features are critical for determining electrolyte bulk properties and how these properties are interrelated. It also provides a ready platform for the rapid characterization of new solvents and salts for electrolyte formulations. Most electrolyte-related research adopts an entirely empirical approach to electrolyte optimization. In sharp contrast, this work enables battery researchers to develop a strong intuition for electrolyte interactions within the bulk liquid phase....and ultimately will result in a comprehensive compendium of knowledge regarding electrolyte composition-property-battery performance relationships