Accurate Prediction of Key Electrolyte Properties Using a Chemical Physics Approach Based on Ion Solvation

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Novel electrolytes are playing an increased role in portable energy systems such as rechargeable batteries (e.g., lithium-ion cells). As the demand for improved performance of these system increases, there is a corresponding need to gain further understanding of the molecular-scale interactions that are the basis for a spectrum of electrolyte properties, such as physical, transport, and thermodynamic quantities. This work has produced an accurate model for electrolyte properties based on an associative form of the Mean Spherical Approximation (AMSA) description of molecular properties and interactions. Complementing the AMSA framework are molecular-based governing equations that express the effect of the molecular environment on various transport properties. The overall model is denoted as the Advanced Electrolyte Model, AEM. Effects from ion solvation are explicitly considered as well as ion-ion interactions, such as ion pairs and triples. The model applies equally to aqueous and nonaqueous systems, multi-solvent systems, and has shown impressive accuracy over wide ranges of solvent composition, solute concentration, and temperature. Although the immediate application of this work is modeling electrolytes for lithium-ion batteries, other potential applications abound. Properties predicted by the model include electrolyte conductivity, viscosity, density, ionic diffusivity, solvation numbers, activity coefficients, and others. Modeling results will be compared to experimental data for an assortment of electrolyte systems, showing that in many cases the average accuracy of the AEM is within 5-10% of experimental values.