Data Driven Development of Binary IL-IL Systems

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ILs are a novel class of salts that exist as liquids at room temperature and possess several favorable properties including high conductivity, low volatility, and high thermal and electrochemical stability. In recent years, binary and ternary IL systems have demonstrated great potential for electrochemical applications including electrolytes for non-lithium batteries, super-capacitors, dye sensitized solar cells and thermo-electrochemical cells. Yet, the vast design space of ILs which includes over one million pure ILs and over 10^{12} and 10^{18} potential binary and ternary combinations (respectively) makes experimental characterization of this space practically infeasible and limits the development of new IL systems.

Accordingly, the design of new IL systems with enhanced electrochemical properties such as high conductivity, ion selective transport, and low viscosity calls for the development of new computational tools. This research centers on developing new binary IL-based systems for electrochemical energy storage combining machine learning and data science informed by the NIST Ionic Liquids Database. This comprehensive database hosts thermodynamic, thermochemical, and transport properties of over 19,000 IL mixtures, with over 700,000 data points aggregated from peer-reviewed literature. Leveraging this data, we identify key structure-property relationships for binary IL mixtures connecting factors such as anions, cations, and electrolyte composition to properties including viscosity, density, and excess molar volume.