Using Machine Learning to Predict Ionic Conductivity of Ionic Liquid Mixtures

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One of the fascinating aspects of ionic liquids is that a large number of ionic liquids can be designed, in principle, leveraging the chemical space of cations, anions, and substituents on these ions. Although this is an attractive strategy, synthesis and subsequent purification to obtain high-purity ionic liquids for thermophysical property measurements can be challenging. On the other hand, a large number of ionic liquids synthesized thus far offers a tremendous opportunity to form ionic liquid-ionic liquid mixtures for fine tuning ionic liquid properties. Measurement of various thermophysical properties can be a daunting task in itself due to an explosion in the number of such mixtures that can be envisioned coupled with obtaining such data as a function of temperature. Machine learning approaches are ideally suited for such applications, if a reasonably large database of measured properties is available. In this presentation, we demonstrate how we make use of the NIST ILThermo Database for ionic liquids to develop machine learning models that are capable of predicting ionic conductivity of ionic liquid-ionic liquid and ionic liquid-solvent systems. We also address methodological challenges in developing machine learning models for predicting mixtures properties.