Discovering High Conductivity Imidazolium-Based Ionic Liquid Mixtures using Artificial Neural Network

Pratik Dhakal[S] and Jindal Shah [C]
School of Chemical Engineering, Oklahoma State University, Stillwater, OK, U.S.A.
Jindal.shah@okstate.edu

Ionic liquids are room temperature ionic solvents characterized by low volatility, designer tunability, high thermal and electrochemical stability. These properties make ionic liquids ideal candidates for the replacement of organic solvents as electrolytes in Li-ion batteries. Despite their favorable attributes, high viscosity of many ionic liquids is a hindrance to exploiting their full potential for battery applications. One way to tackle this challenge is to develop novel ionic liquids by altering the identity of the cation, anion, or substituents on the ions. The enormous chemical space for such a manipulation is extremely difficult, if not impossible, to navigate efficiently via experimental or molecular simulation-based approaches. In such instances, machine learning techniques offer an exciting alternative, if sufficient data is available to train a model.

In this presentation, we will describe our efforts at developing a machine learning model based on the ionic conductivity data obtained from the NIST ILThermo Database. A feed forward artificial neural network (FFAAN) comprised of an input layer, a hidden layer and an output layer is obtained from the data on ~100 ionic liquids. We will demonstrate that the FFAAN is able to capture the data with a high degree of accuracy over five orders of magnitude. The machine learning model is then used to predict the ionic conductivity data for ~1200 pure ionic liquids obtained by combining the unique cations and anions in the database. We will show how the machine learning model can be employed to predict the ionic conductivity for ~840,000 ionic liquids. The validity of such predictions will be demonstrated by comparing the ionic conductivity of those binary ionic liquids for which experimental data is available. Furthermore, we will report on 5000 potential binary ionic liquid-ionic liquid mixtures for which there exists a possibility for obtaining ionic conductivity higher than those of the pure ionic liquids making up the binary ionic liquid mixtures.