EXTENSION OF THE CL&P IONIC LIQUID FORCE FIELD TO PYRAZOLIUM IONIC LIQUIDS

Adam Sturlaugson*
Department of Chemistry
University of Sioux Falls
Sioux Falls, SD 57105
*Corresponding author email: adam.sturlaugson@usiouxfalls.edu

ABSTRACT

In 1992, Wilkes and Zaworotko synthesized the first air- and water-stable ionic liquids. Since then, their imidazolium-based ionic liquids have been the most studied class of ionic liquids, both experimentally and computationally. Most molecular dynamics simulations of imidazolium ionic liquids have been performed using a force field developed by Canongia Lopez and Padua (the CL&P force field), which has been shown to model the liquid structure well. Since the original publication of the CL&P force field in 2004, it has been extended to include other non-imidazolium ionic liquid classes. Here, an extension of the CL&P force field to include pyrazolium-based ionic liquids is presented. While they have only a very minor presence in the scientific literature, pyrazolium ionic liquids are easily synthesized and have structural variations amenable to the investigation of structure-property relationships in ionic liquids. If experimentally validated, this pyrazolium force field could serve a key role in helping answer some of the outstanding questions regarding structure-property relationships in ionic liquids.