Exploring the Impact of Cation Diversity on Properties of Bis(trifluoromethylsulfonyl)imide Ionic Liquids

Pranav Thacker[1, S], Jiaying Jin[1], Mariam Y. Balogun[1], Louise M. Cañada[1] and Joan F. Brennecke[1, C]

[1]*McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX, U.S.A.*
jfb@che.utexas.edu

This research delves into the multifaceted relationship between cation diversity and ionic liquid (IL) properties, offering a fresh perspective for a wide array of potential applications. Within this expansive exploration, a diverse range of cations is examined, encompassing variations in structure, charge localization, heteroatom, and an extensive spectrum of characteristics. Cations are paired with a common anion, bis(trifluoromethylsulfonyl)imide ([Tf2N]–), in order to analyze their influence on key properties, including thermal stability, density, viscosity, and CO_2 and N_2 solubility. In addition to a comprehensive physicochemical property analysis, the study incorporates fundamental electrochemical characterizations—ionic conductivity and cyclic voltammetry—enhancing our understanding of the electrochemical behavior of these diverse ILs. Leveraging DFT (*ab initio*) solvent-phase calculations, the research also unveils a broad pK_a range for the cation candidates, further elucidating their ionization behavior within the IL framework. In conclusion, this study serves as a versatile resource for researchers and engineers seeking to optimize ILs for their unique applications. By analyzing the relationship between cation choice and IL properties, this research paves the way for tailoring solutions across a multitude of domains. The findings not only provide insights into specific applications but also contribute to the broader understanding of how to harness cation diversity for versatile and adaptive solutions.