

Abstract Submitted
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Ion shape effect on dynamics of ionic liquids HONGJUN LIU, EDWARD MAGINN, University of Notre Dame — Ionic liquids (ILs) are a group of salts composing of an organic cation and organic or inorganic anion with melting points below 100 °C and have many suitable properties, such as negligible vapor pressure, low flammability, high ionic conductivity and high thermal stability for various applications. Moreover, a great number of ILs with a variety of physical and chemical properties can be synthesized from a combination of different cations (most differently substituted imidazolium, pyridinium, and quaternary ammonium or phosphonium ions) and anions. One can judiciously select from a multitude of ILs to suit a specific application, where the concept of designer solvent comes from. To expedite the development process of target ILs, it is crucial to understand the relationship between ion shape and dynamics of ILs. We studied a wide range of ILs with different ion shape pairings and found the planar-planar paired ILs have a better dynamics as a whole.

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