Anion-based magnetic ionic liquids: from non-polarizable to polarizable force fields

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Magnetic ionic liquids (MILs) are a new class of ionic liquids that contain a paramagnetic atom (e.g., iron, cobalt, dysprosium) in their cation or anion structure and yield a magnetic response in the presence of an external magnetic field. These compounds exhibit the same exceptional and tunable properties as ILs, such as negligible vapor pressure, low flammability, and high thermal and chemical stability.[1] In addition, the magnetic response enhances their transport properties, such as increasing ion diffusion and consequently reducing viscosity.[2] Moreover, experimental results show that MILs can be effortlessly recycled by magnetic separation, saving extraction steps, and reducing the use of organic compounds.[3]
Since 2004, MILs have been emerged for a wide range of applications such as gas capture, environmental remediation, PET depolymerization, food safety analysis, and biomedical needs.[1,3] However, there are few atomistic level studies due to the lack of force fields for these anion species.
The aim of this work is to establish a non-polarizable and a polarizable force field for (FeX_4)-based MILs, where X = Cl or Br atoms, and to investigate thermodynamic, transport and structural properties using molecular dynamics (MD) simulations (Figure 1). This study will help to propose a cost-effective design of MILs and their mixtures to boost their potential applicability and is the starting point for new insights into the nature of these magnetoactive substances.

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FIGURES

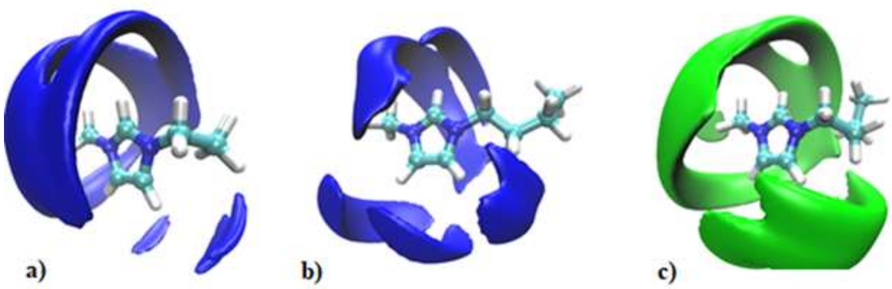

Figure 1: Spatial distribution functions of a) [Emim][$FeCl_4$], b) [Bmim][$FeCl_4$], and c) [Bmim][$FeBr_4$] describing the distribution of [$FeCl_4$] (blue) and [$FeBr_4$] (green) anion around the reference cation at 293.15 K.