Charge Inverted-Ionic Liquids: from Aromatic to Aliphatic Ions

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Salts based on alkali cations and molecular anions usually exhibit high melting point temperatures, while salts based on molecular cations combined with halogen anions are ionic liquids used in many different applications. This problem was addressed in a recent study that compares the properties of a *charge-inverted* IL series (potassium 1alkyl-3-methylcyclopentadienyl, K[C_nC₁Cp]) and their 1-alkyl-3-methylimidazolium chloride counterparts, [C_nC₁im]Cl). [1] In this work, we studied by molecular dynamics simulations new charge-inverted ILs based on potassium tetraalkylborate, K[B_{n n n}] as mirror images of well-known ionic liquids of the tetraalkylammonium chloride family, [N_{n n n}]Cl, where n = 2, 4, 6, 8, and 10. Structural and coordination differences between the ILs containing aromatic and aliphatic molecular ions will be discussed in this presentation.

References:

[1] Cruz, T. F. C. et al. Faraday Discuss. **2017**, doi: 10.1039/c7fd00139h.

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