Structure and Dynamics of ionic liquids from first principles simulations: Effects of dispersion corrected density functionals and charge density cutoff

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The thermodynamics, structural and transport properties of an Ionic liquid(IL) were investigated through first principles molecular dynamics simulations. The simulations were carried out using different generalized gradient approximation functionals and the charge density cutoff in the isobaric-isothermal and canonical ensembles. The effects of dispersion interactions on the various properties of cations and anions were investigated. Thermodynamic properties of IL are sensitive to the details of the electronic structure calculations. Subsequently, the calculations were extended to the time dependent vibrational spectroscopy and preliminary results were discussed in terms of correlation between spectral signature and hydrogen bond dynamics.

References:

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