Multiscale simulations on the structure and dynamics of ionic liquids

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Ionic liquids (ILs) are a class of molten salts with low melting point, which are typically but not exclusively composed of organic cations and inorganic anions. This class of salts showed promising applications in the fields of electrochemistry, catalysis, biochemistry etc. Nevertheless, there is a lack of fundamental understanding about the structures and the dynamics properties of ILs. We aim at a multiscale modelling approach, where we describe the system from the electronic scale up to the atomistic scale (from electron-correlating wavefunction based methods via DFT to classical MD) in a self-consistent way.[1] Here we present first results obtained for the benchmark system 1,3-dimethylimidazolium chloride ([DMIM][Cl]), like structures and energy profiles obtained on the post-HF level.[2] In addition, partial charge is an important parameter in classical force fields, employed in molecular dynamics simulations. We also discuss here the charge scaling idea and the results determined on different level of theory, from electronic to the atomistic scale, with various protocols.[3]

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