Ionic Liquids in classical MD simulations

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In recent years Room Temperature Ionic Liquids (RTIL) have become a major subject in various fields of research. The main feature of these salts which consist of organic bulky cations and organic or anorganic anions is their low melting point and vapour pressure. Unfortunately a complete understanding of the properties is lacking and also an appropriate picture of the processes occuring in the liquid bulk. A good tool to investigate this situation is a classical molecular dynamics (MD) simulation. However the basis of every MD simulation is a reliable force field which is not available for most of the known RTIL. Therefore we aim on a method to efficiently derive force fields from scratch with the help of quantum chemical, Car-Parrinello and MD simulations. The talk will shortly present some of the currently studied ionic liquids and an example for a refinement process of a force field for [MMIM][Cl].