Ionic Liquids
Tackling Little Beasts in Molecular Dynamics simulations

Ionic liquids belong to a class of rediscovered solvents. They can easily be tuned to the desired properties just by modifying the cation or anion. However the nature of this liquids is not understood completely. A powerful tool to investigate the statics and dynamics of ionic liquids are Molecular Dynamics simulation, that require a force field to describe the inter and intramolecular interactions within the solvent. Unfortunately reliable force fields exists just for special combinations of anion and cation. We aim on developing an efficient way to parameterize force fields for ionic liquids with the help of different computational methods on several scales, starting from highly accurate post Hartree-Fock calculations via ab-initio Car-Parrinello Molecular Dynamics simulations and finally ending up in classical Molecular Dynamics simulations.