MD Simulations of Ionic Liquids: Relations Between Ion Tranport, Thermodynamics and Ion Size

Oleg Borodin, University of Utah, Salt Lake City, UT & Wasatch Molecular Inc.

Classical molecular dynamics (MD) simulations have been performed on a wide set of ionic (IL) liquids containing alkyl-imidazolium, pyrrolidinium, pyridinium, piperidinium and morpholinium cations and BF4-, PF6- , CF3SO3, CF3BF3, CH3BF3, dicyanamide, bis(trifluoromethane sulfonyl) imide and nitrate cations. Many-body polarizable force field has been used in simulations of ionic liquids. MD simulations predicted density, ion self-diffusion coefficient, conductivity and viscosity in good agreement with available experimental data. This presentation will focus on the correlation between ion transport in ionic liquids with thermodynamic data (enthalpy of vaporization, cation-anion dimer energies) and structure of ionic liquids. A nonlinear relation between size of the anions and ionic transport will also be analyzed in details.