Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Atomistic polarizable force field for molecular dynamics simulations of azide anion containing ionic liquids and crystals.[1] OLEG STAROVOYTOV, The University of Utah, JUSTIN HOOPER, Wasatch Molecular Incorporated , OLEG BORODIN, GRANT SMITH, The University of Utah — Atomistic polarizable force field has been developed for a number of azide anion containing ionic liquids and crystals. Hybrid Molecular Dynamics/Monte Carlo (MD/MC) simulations were performed on methylguanazinium azide and 1-(2-butynyl)-3-methyl-imidazolium azide crystals, while 1-butyl-2,3-dimethylimidazolium azide and 1-amino-3-methyl-1,2,3-triazolium azide ionic liquids were investigated using MD simulations. Crystal cell parameters and crystal structures of 1-(2-butynyl)-3-methyl-imidazolium azide were found in good agreement with X-ray experimental data. Density and ion transport of 1-butyl-2,3-dimethylimidazolium azide predicted from MD simulations were in good agreement with experiments. Details of the ionic liquid structure and relaxation mechanism will be discussed.

[1]Financial support from Air Force Office of Scientific Research (FA9550-09-C-0110) is acknowledged

Oleg Starovoytov
The University of Utah

Date submitted: 19 Nov 2009 Electronic form version 1.4