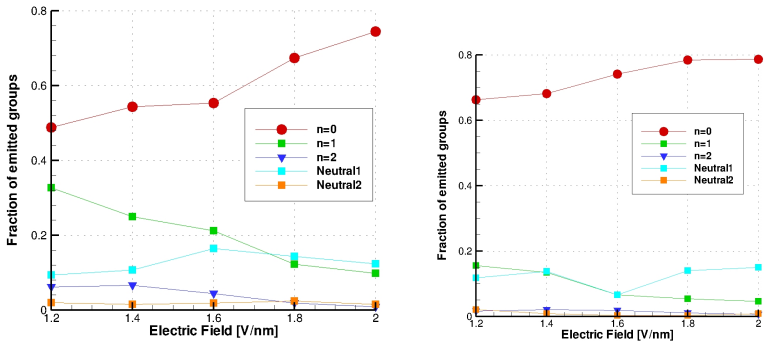
Significant Research Results Write up - MACEEP Project –
July 2, 2012, Debbie Levin

Modeling of Fundamental Processes in Electrospray Systems

Can coarse grained intermolecular potentials represent the physics of an ionic liquid/Taylor cone spray emission? One green IL propellant is the 1-ethyl-3-methylimidazolium/ tetrafluoroborate molecule also known as EMIM-BF_4. This system is or interest to the Air Force because the large cation is accelerated in an external electric field. Our recently published large simulations (A. Borner, Z. Li, and D. Levin, "Modeling of an Ionic Liquid Electrospray using Molecular Dynamics with Constraints," *The Journal of Chemical Physics*, Vol. 123, 124507 (2012); doi: 10.1063/1.3696006) shows that using such an intermolecular potential we can simulate an extruded system sufficiently large to capture the distribution of solvated ions. The simulations provide the first type of information to show the fundamental, molecular structure of ion clusters that will be formed for different magnitudes of the electric field. The majority of ions extruded are non-solvated (i.e., generate more thrust), and, as the electric field strength increases, the proportion of single ions also increases. The atomistic simulations also show that larger solvated ions break apart when formed in higher electric fields.



Solvated and non-solvated ions distribution: (LHS) shows the positive ions of the form $(EMIM\text{-}BF4)_nEMIM^+$ and (RHS) shows negative ions of the form $(EMIM\text{-}BF4)_nBF4^-$ where n is the number of neutral cation/anion pairs.