Abstract Submitted
for the DFD17 Meeting of
The American Physical Society

Molecular modeling of field-driven ion emission from ionic liquids

FEI ZHANG, YADONG HE, RUI QIAO, Virginia Tech — Traditionally, operating electrosprays in the purely ionic mode is challenging, but recent experiments confirmed that such operation can be achieved using room-temperature ionic liquids as working electrolytes. Such electrosprays have shown promise in applications including chemical analysis, nanomanufacturing, and space propulsion. The mechanistic and quantitative understanding of such electrosprays at the molecular level, however, remain limited at present. In this work, we simulated ion emission from EMIM-PF6 ionic liquid films using the molecular dynamics method. We show that, when the surface electric field is smaller than $\sim$1.5V/nm, the ion emission current predicted using coarse-grained ionic liquid model observes the classical scaling law by J. V. Iribarne and B. A. Thomson, i.e., $\ln(\mathrm{Je}/\sigma) \sim \mathrm{En}^{1/2}$. These simulations, however, cannot capture the co-emission of cations and anions from ionic liquid surface observed in some experiments. Such co-emission was successfully captured when united-atom models were adopted for the ionic liquids. By examining the co-emission events with picosecond, sub-angstrom resolution, we clarified the origins of the co-emission phenomenon and delineate the molecular events leading to ion emission.

Fei Zhang
Virginia Tech

Date submitted: 25 Jul 2017 Electronic form version 1.4