Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Atomistic Simulations of Ternary Polymer Electrolytes Containing Ionic Liquids: Ion Transport and Viscoelastic Behavior SANTOSH MOGURAMPELLY, VENKAT GANESAN, Univ of Texas, Austin — Influence of the $BMIMPF_6$ ionic liquid on ion transport and viscoelastic properties of ternary polymer electrolytes containing polyethylene oxide solvated with $LiPF_6$ salt and the underlying mechanisms are investigated. By employing atomistic molecular dynamics and trajectory extended kinetic Monte Carlo simulation techniques, we observe enhanced ionic mobilities and conductivities of the $PEOLiPF_6$-$BMIMPF_6$ ternary electrolytes upon the addition ionic liquid into the $PEOLiPF_6$ binary electrolyte. The dispersion of the $BMIMPF_6$ ionic liquid into the $PEOLiPF_6$ electrolyte is found to (a) promote dissociation of existing $LiPF_6$ ion-pairs and (b) slightly accelerate the polymer segmental dynamics. Together, these effects are observed to collectively give rise to an increase in ionic mobilities and conductivities of the ternary polymer electrolyte. On the other hand, Rouse analysis reveals that the storage and loss modulus of the ternary polymer electrolytes are coupled to their ion conducting properties.

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Date submitted: 05 Nov 2015 Electronic form version 1.4