

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Understanding glass formation and ion transport in polymeric ionic liquids using computer simulations TARAK PATRA, JUNHONG YANG, YIZ CHENG, DAVID SIMMONS, The University of Akron — Polymeric ionic liquids (PILs) are very promising materials to enable more environmentally stable high density energy storage devices. Realization of PILs providing high environmental and mechanical stability while maximizing ion conductivity would be accelerated by an improved molecular level understanding of their structure and dynamics. Extensive evidence suggests that both mechanical properties and ion conductivity in anhydrous PILs are intimately related to the PIL's glass formation behavior. This represents a major challenge to the rational design of these materials, given that the basic nature of glass formation and its connection to molecular properties remains a substantial open question in polymer and condensed matter physics. Here we describe coarse-grained and atomistic molecular dynamics simulations probing the relationship between PIL architecture and interactions, glass formation behavior, and ion transport characteristics. These studies provide guidance towards the design of PILs with improved stability and ion conductivity for future energy applications.

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Date submitted: 12 Nov 2016

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