Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Multi-scale simulations of Na2S + SiS2 glassy electrolyte SCOTT BECKMAN, ANIRUDDHA DIVE, CLARENCE KING, Washington State University, STEVE MARTIN, Iowa State University, SOUMIK BANERJEE, Washington State University — Developing solid electrolytes with high ionic conductivity is a significant challenge. Here we explore sulfide glasses as potential electrolytes. A classical molecular dynamics approach was applied to evaluate the structures and ionic conductivity of a wide range of xNa2S – (1-x) SiS2 glassy electrolytes. Due to their amorphous nature, various starting configurations obtained using a typical melt-quench technique were explored to gather statistically reasonable structures. In order to validate the model, the results from the pair distribution functions for [0.5Na2S – 0.5SiS2] were compared with structure factor data from experiments. Finally, ionic conductivity was calculated for varying compositions to identify the most promising electrolytes. To scale up the calculations, allowing for the determination of interface properties and large scale calculations, a kinetic Monte Carlo simulation is developed to work in conjunction with the molecular dynamics calculations. Using this approach, it is possible to model the conductivity in these glasses from the atomic level to the macroscale.

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Date submitted: 11 Nov 2016 Electronic form version 1.4