Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Structure and interface properties of the electrolyte material $Li_4P_2S_6$[1] ZACHARY D. HOOD, Oak Ridge National Lab., CAMERON KATES[2], N. A. W. HOLZWARTH, Wake Forest U. — $Li_4P_2S_6$ has been identified in several high temperature preparations of lithium thiophosphate electrolytes as a synthesis or decomposition product. Its characteristic P−P bond may be partly responsible for its relative stability. Early structural analysis[3] found the P sites to be disordered. Our previous simulations,[4] found a related low energy structure with ordered P sites. We report here a re-examination of the simulation results and new X-ray measurements which indicate that the lowest energy structure of $Li_4P_2S_6$ is different from that determined in previous analysis. Ionic conductivity and thermal stability are also reported. In addition to examining the bulk electrolyte, we have simulated idealized interfaces of $Li_4P_2S_6$ and lithium metal representing an electrolyte/anode system.

[1]Supported by NSF grant DMR-1105485.
[2]Currently attending the Pratt School of Engineering at Duke U.
[3]R. Mercier *et. al.*, *J. Solid State Chem.* **43** 151 (1982)
[4]N. A. W. Holzwarth, *J. Power Sources* **196** 6970 (2011)

Natalie A Holzwarth
Wake Forest Univ

Date submitted: 13 Nov 2014 Electronic form version 1.4