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Surface Structure and Stability in Li_3PS_4 and Li_3PO_4 Electrolytes from First Principles[1] NICHOLAS LEPLEY, N.A.W. HOLZWARTH, Wake Forest University — Crystalline solid electrolyte materials continue to show considerable promise for lithium ion battery applications. Recent experiments on these materials[2] suggest that in some cases surface effects may play a significant role with regard to both stability and ionic conductivity. In this study, we extend our previous modeling work[3] to an examination of idealized surfaces of several phases of Li_3PX_4 (X=O,S). Our preliminary results suggest that energy contributions from the surface affect the relative phase stability in Li_3PS_4, although this is not observed in the phosphate analogue. Our presentation will focus on surface energies and structures, as well as examining the calculated stability of the interface between the electrolyte and lithium metal.

[1]Supported by NSF Grant DMR-1105485.
[2]Chengdu Liang, ORNL, (private communication).
[3]N. A. W. Holzwarth, N. D. Lepley, Y. A. Du, *J. Power Sources* **196**, 6870 (2011).

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