Abstract Submitted
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First principles modeling of interfaces of lithium (thio) phosphate solid electrolytes and lithium metal anodes[1] N.A.W. HOLZWARTH, N.D. LEPLEY, A.N.M. AL-QAWASMEH, C.M. KATES, Wake Forest University — Computer modeling studies show that while lithium phosphate electrolytes form stable interfaces with lithium metal anodes, lithium thiophosphate electrolytes are typically structurally and chemically altered by the presence of lithium metal. On the other hand, experiments have shown[2] that an electrochemical cell of $Li/Li_3PS_4/Li$ can be cycled many times. One possible explanation of the apparent experimental stability of the $Li/Li_3PS_4/Li$ system is that a stabilizing buffer layer is formed at the interface during the first few electrochemical cycles. In order to computationally explore this possibility, we examined the influence of "thin film" buffer layers of Li_2S on the surface of the electrolyte. Using first principles techniques,[3] stable electrolyte-buffer layer configurations were constructed and the resulting Li_3PS_4/Li_2S and Li_2S/Li interfaces were found to be structurally and chemically stable.

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[2]Z. Liu, W. Fu, *et. al.*, *J. Am. Chem. Soc.* **135** 975-978, (2013).
[3]N. D. Lepley, N. A. W. Holzwarth, Y. A. Du, *Phys. Rev. B* **88**, 104103 (2013).

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