

First Principles Modeling of the Interface Between a Solid State Lithium Thiophosphate Electrolyte and a Lithium Metal Anode

To cite this article: Natalie A. W. Holzwarth and Nicholas D. Lepley 2013 *Meet. Abstr.* **MA2013-02** 563

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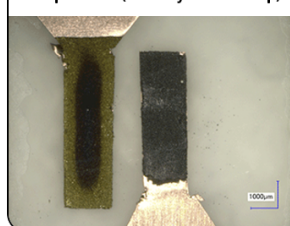
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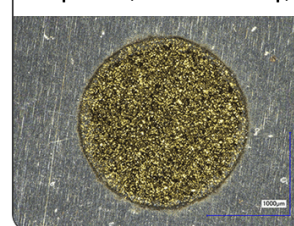
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**First principles modeling of the interface between
a solid state lithium thiophosphate electrolyte
and a lithium metal anode**

N. A. W. Holzwarth and N. D. Lepley
Department of Physics, Wake Forest University
Winston-Salem, NC 27109, USA

Recently, there has been progress in improving the conductivity and stability of solid electrolytes such as Li_3PS_4 . [1] We report the results of first principles computer modeling studies of ideal Li_3PS_4 electrolyte interfaces with metallic Li anodes.

For a variety of interface configurations, computer modeling studies show that Li_3PS_4 surfaces are structurally and chemically altered by the presence of Li metal. On the other hand, experiments have shown [1] that an electrochemical cell of $\text{Li}/\text{Li}_3\text{PS}_4/\text{Li}$ can be cycled many times. One possible explanation of the apparent stability of the Li_3PS_4 electrolyte/Li metal interface, is that a stable thin buffer layer is formed during the first few cycles. In order to computationally explore this possibility, we modeled a “thin film” buffer layer of Li_2S on the surface of the electrolyte. Using first principles techniques described in previous work, [2] stable electrolyte-buffer layer configurations were found. Results for the idealized configurations indicate that a thin film of Li_2S can provide a protective buffer layer to stabilize the interface between the Li_3PS_4 electrolytes and Li metal anodes.

Acknowledgments

This work was supported by NSF Grant DMR-1105485. Computations were performed on the Wake Forest University DEAC cluster, a centrally managed resource with support provided in part by the University. Helpful discussions with Chengdu Liang and Nancy Dudney of Oak Ridge National Laboratory are gratefully acknowledged.

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