Abstract Submitted
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Modeling solid electrolyte/electrode interface stability using first principles calculations[1] NICHOLAS LEPLEY, N. A. W. HOLZWARTH, Wake Forest University — The formation of a stable interface between electrode and electrolyte materials is a necessary property for batteries in general and for Li-ion batteries in particular. We present a framework for understanding and predicting the electrochemical stability of electrode/electrolyte interfaces based on density functional theory calculations. Within this framework, we have extended our previous work[2] to include quantitative results for the solid-solid interface energy of the Li_3PS_4/Li, Li_3PO_4/Li, Li_2S/Li, Li_2O/Li, and Li_3PS_4/Li_2S interfaces. We show that under local equilibrium conditions the interface energy appears to be a good indicator of the stability of the interface. While the results we present are focused on the interface between Li-ion solid electrolytes and Li metal we expect the method to be applicable to other interface systems.

[1]Supported by NSF Grant DMR-1105485
[2]N. D. Lepley, N. A. W. Holzwarth, and Y. A. Du, Phys. Rev. B **88**, 104103 (2013).

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