

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**A formalism for modeling solid electrolyte/electrode interfaces using first principles methods**<sup>1</sup> NICHOLAS LEPLEY, Wake Forest Univ, NATALIE HOLZWARTH, Wake Forest University — We describe a scheme based on the interface energy for analyzing interfaces between crystalline solids, quantitatively including the effect of lattice strain. This scheme is applied to the modeling of likely interface geometries of several solid state battery materials including Li metal,  $\text{Li}_3\text{PO}_4$ ,  $\text{Li}_3\text{PS}_4$ ,  $\text{Li}_2\text{O}$ , and  $\text{Li}_2\text{S}$ . We find that all of the interfaces in this study are stable with the exception of  $\text{Li}_3\text{PS}_4/\text{Li}$ . For this chemically unstable interface, the partial density of states helps to identify mechanisms associated with the interface reactions. We also consider the case of charged defects at the interface, and show that accurately modeling them requires a careful treatment of the resulting electric fields. Our energetic measure of interfaces and our analysis of the band alignment between interface materials indicate multiple factors which may be predictors of interface stability, an important property of solid electrolyte systems.

<sup>1</sup>Supported by NSF Grant DMR-1105485 and DMR-1507942

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Date submitted: 06 Nov 2015

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