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$_3$PS$_4$/Li, Li$_3$PO$_4$/Li, Li$_2$S/Li, Li$_2$O/Li, and Li$_3$PS$_4$/Li$_2$S 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.

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