Abstract Submitted
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**High Throughput Computational Discovery of Intermetallic Anodes for Li Batteries**[1] SCOTT KIRKLIN, Northwestern University, CHRIS WOLVERTON — We have developed a framework to perform high-throughput computational screening of intermetallic compounds as candidates for Li battery anodes. We have used our method to calculate, from density functional theory (DFT), more than 5000 anode lithiation reactions, based on more than 100 intermetallic compounds. We have specifically focused on the 3d-transition metal silicides, nidtrides and phosphides. Given the set of DFT total energies for all compounds, the reaction path upon lithiation is predicted using the recently-developed grand canonical linear programming (GCLP) method. The anode performance is then characterized by the cell potential vs lithium metal, energy density and volume expansion. The accuracy of this approach is first validated for pure silicon, and then extended to binary intermetallic compounds. Based on the results of these calculations, future experimental study can be guided toward systems with promising thermodynamic properties.

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