

Abstract Submitted
for the 4CS19 Meeting of
The American Physical Society

Finding Ways to Stabilize Potential New Superalloys TYLER WHITAKER, BRAYDEN BEKKER, GUS HART, Brigham Young University — The ability to create something new and interesting depends heavily on the materials available to us. The search for new superalloys provides many opportunities in energy production and structural integrity. By using high-throughput methods, we are able to find potential quaternary additions to known metastable ternary superalloys. We use density functional theory (DFT) to find a list of elements that could stabilize each ternary alloy. We then use a machine-learned interatomic potentials (called moment tensor potential, or MTP) to explore the stability of the superalloy phases in the quaternary systems found from DFT. Through these steps, we are able to find the quaternary compositions the most stable superalloy phases when synthesized.

Tyler Whitaker
Brigham Young University

Date submitted: 12 Sep 2019

Electronic form version 1.4