Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

High-throughput calculations of pressure-induced phase transitions in tungsten nitride[1] MICHAEL MEHL, Naval Research Laboratory, Washington DC, DANIEL FINKENSTADT, United States Naval Academy, Annapolis MD, GUS HART, Brigham Young University, Provo UT, STEFANO CURTAROLO, Duke University, Durham NC — We have previously[2] used high-throughput electronic structure calculations[3] to determine the ground state structures of the tungsten-nitride system as a function of composition. In doing this, we found many structures with are close to the W-N convex hull and apparently metastable. The question then arises if any of these structures can be stabilized under pressure. To test this, we have determined the ground state hull as a function of pressure up to 50 GPa. We find that the structures on the hull change with pressure. We discuss some of the more interesting structures, and show how the choice of density functional changes our predictions.

[1]Partial support from US-ONR and US DoD HPC
[2]M. Mehl *et al.*, arXiv:1403.2762 [cond-mat.mtrl-sci] (2014)
[3]S. Curtarolo *et al.*, http://materials.duke.edu/aflow.html

Michael Mehl
Naval Research Laboratory, Washington DC

Date submitted: 13 Nov 2014 Electronic form version 1.4