Abstract Submitted
for the MAS15 Meeting of
The American Physical Society

Ti-Ni Crystal Structure Prediction by Minima Hopping Method
ADAM PAYNE, IRAIS VALENCIA-JAIME, GUILLERMO AVENDAO-FRANCO, RAYMUNDO ARROYAVE, ALDO ROMERO, Department of Physics and Astronomy, West Virgnia University, Morgantown WV 26506 — Titanium alloys have wide applications from industry to medicine due to their unique properties of shape memory and superelasticity. While it is known that these amazing properties result from an interplay between titaniums low temperature cubic β phase and its high temperature hexagonal phase, the exact nature of this interplay is poorly understood. Investigating how the elastic properties vary with composition is crucial to understanding this mechanism. We have performed a structural search method known as Minima Hopping [1] to identify the ground state structure in thirty-one compositions. We also identify metastable structures, which are of interest because they can be stabilized with the addition of other atoms. We found the convex hull, and have compared it to known experimental and computational results. Elastic, electronic, and energetic properties are computed for the ground state structures using first-principle calculations as implemented in the VASP code. [2] We report the structures with interesting elastic and vibrational properties, and convey several options for future work. [1] Buehler, W. J., R. C. Wiley. No. NOLTR- 61-75. Naval Ordnance Lab White Oak MD, 1961 [2]S. Goedecker, The J of chem phys 120,9911 (2004)

Adam Payne
Department of Physics and Astronomy, West Virgnia University, Morgantown WV 26506

Date submitted: 02 Oct 2015 Electronic form version 1.4