Abstract Submitted for the MAR07 Meeting of The American Physical Society

Ti-V alloy phase diagram: DFT-based cluster approach¹ MICHAEL R. FELLINGER, JOHN W. WILKINS, The Ohio State University, DALLAS R. TRINKLE, University of Illinois-UC — V is an important alloying element for Ti since it stabilizes the high-temperature bcc phase of Ti at lower temperatures, while minimizing the formation of intermetallic compounds [1]. Theoretical determination of the Ti-V phase diagram must take into account structures based on both bcc and hcp lattices over the full V concentration range. With the cluster expansion formalism for alloys [2], DFT calculations determine the energies of all structures necessary for constructing the cluster expansion for the energetics of the alloy. Preliminary results indicate the DFT-based cluster approach determines solubility limits and transformation temperatures that are in good agreement with the experimental phase diagram [3].

 M. J. Donachie, Jr., *Titanium: A Technical Guide.* ASM International: Metals Park, OH (1988).
D. de Fontaine, Solid State Phys. **47**, 33 (1994).
T. B. Massalski, et al., *Binary Alloy Phase Diagrams*, Vol. 2. ASM International: Metals Park, OH (1986).

¹Supported in part by the DOE. We thank R. G. Hennig of Cornell U. for useful discussions.

Michael R. Fellinger The Ohio State University

Date submitted: 20 Nov 2006

Electronic form version 1.4