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Spin-gapless semiconductivity and half metallicity in Heusler alloys

Bradley A. Staten

University of Northern Iowa, bstaten@uni.edu

Pavel V. Lukashev

University of Northern Iowa, pavel.lukashev@uni.edu

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Spin-gapless semiconductivity and half metallicity in Heusler alloys



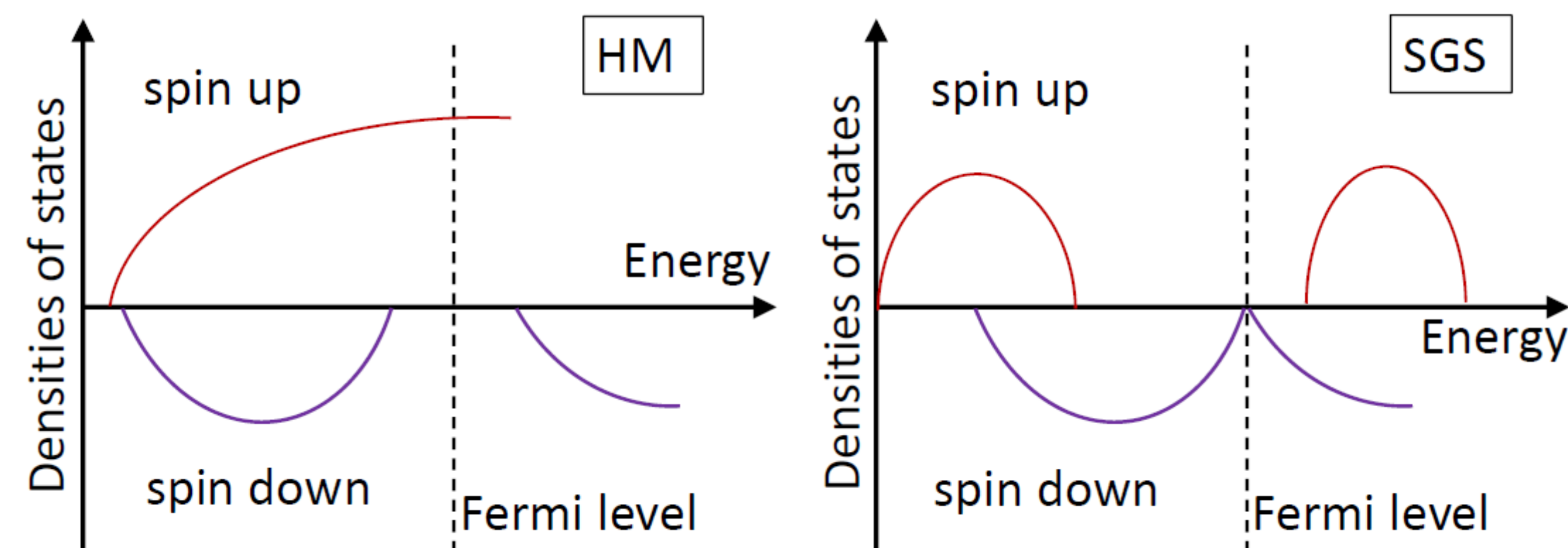
Bradley A. Staten, Pavel V. Lukashev

Department of Physics, University of Northern Iowa, Cedar Falls, Iowa 50614, USA

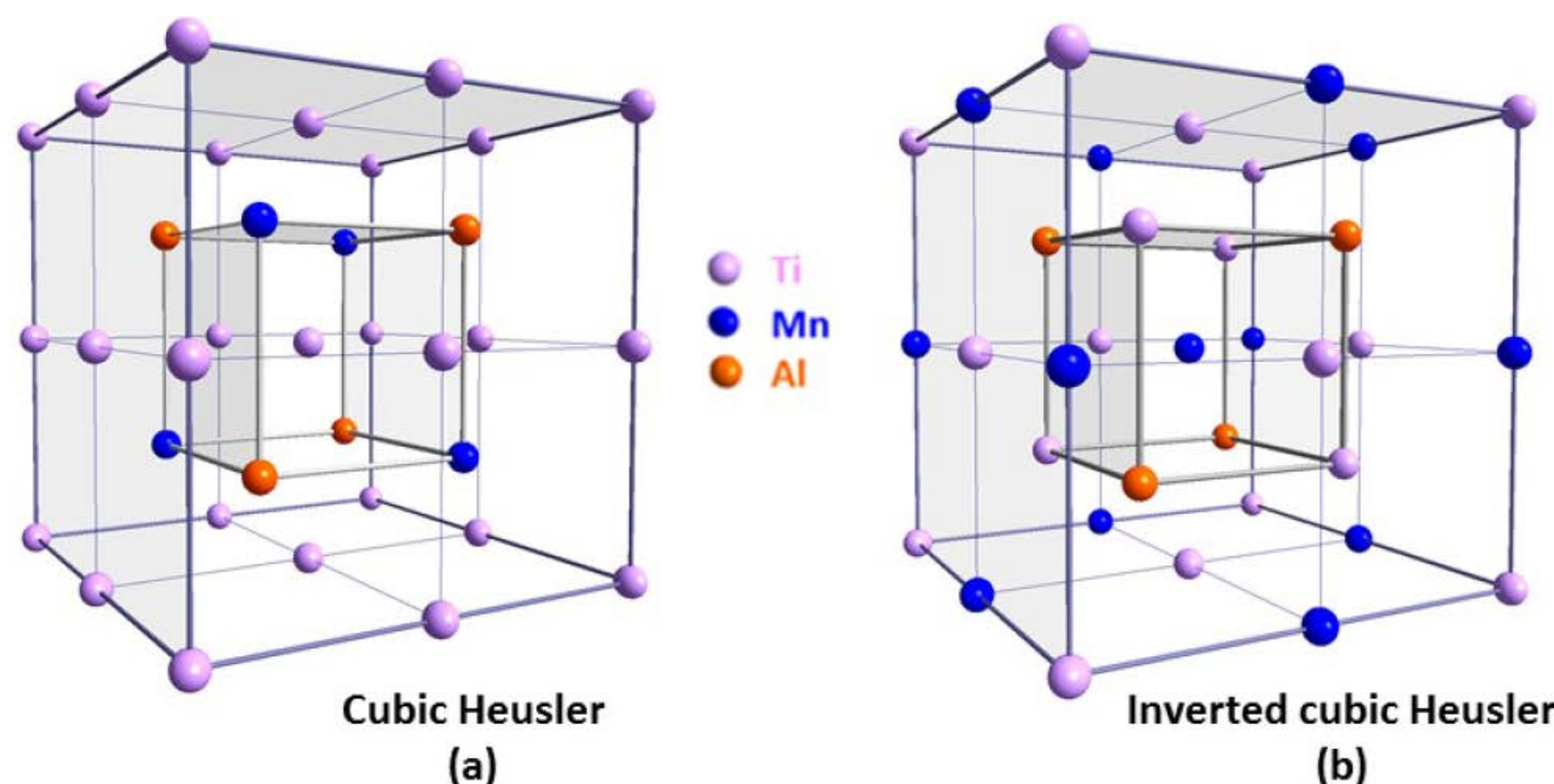


Motivation and Introduction

- ✓ Increasing interest in spin-based electronics (spintronics) has led to a vigorous search for new materials that can provide a high degree of spin polarization in electron transport.
- ✓ Ideal candidate would act as an insulator for one spin channel and a conductor or semiconductor for the opposite spin channel, corresponding to the respective cases of half-metallicity (HM) and spin-gapless semiconductivity (SGS).
- ✓ Recently, an interesting new class of materials, namely spin-gapless semiconductors, have attracted much attention due to potential applications in spintronics.
- ✓ SGS are characterized by a zero band gap in one spin channel and by a finite band gap in the other channel, and therefore are different from ferromagnetic materials with semiconducting electron transport, including dilute magnetic semiconductors



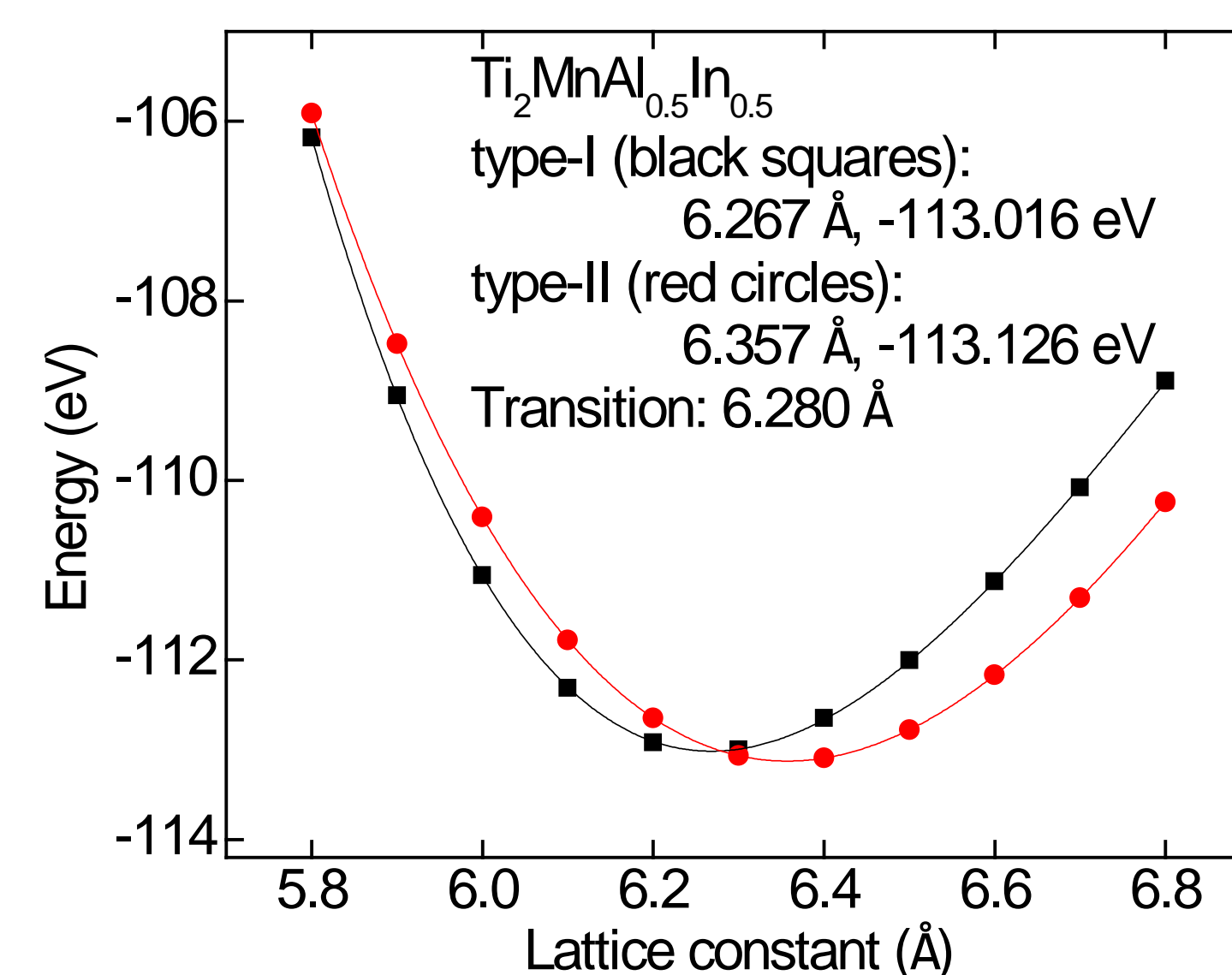
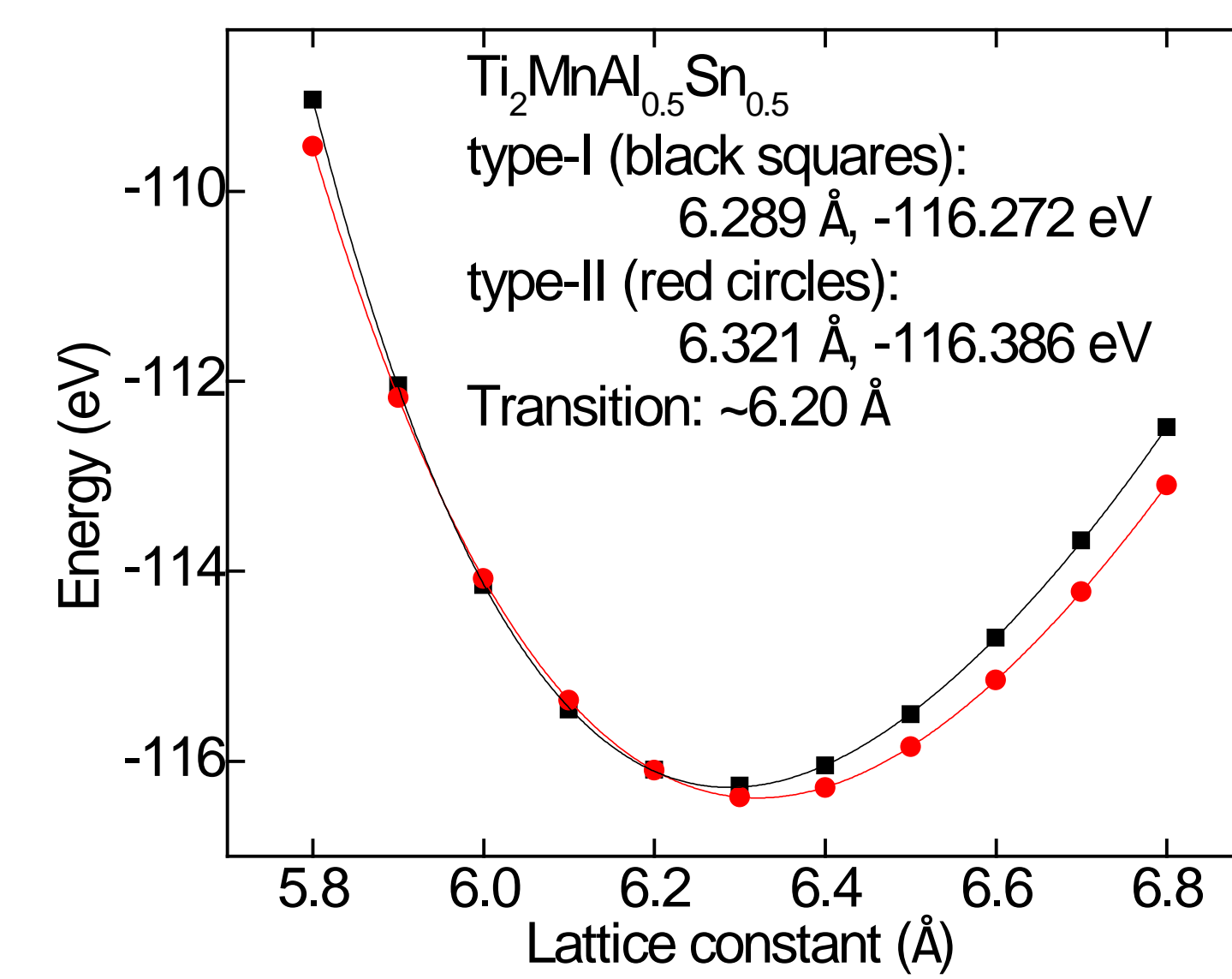
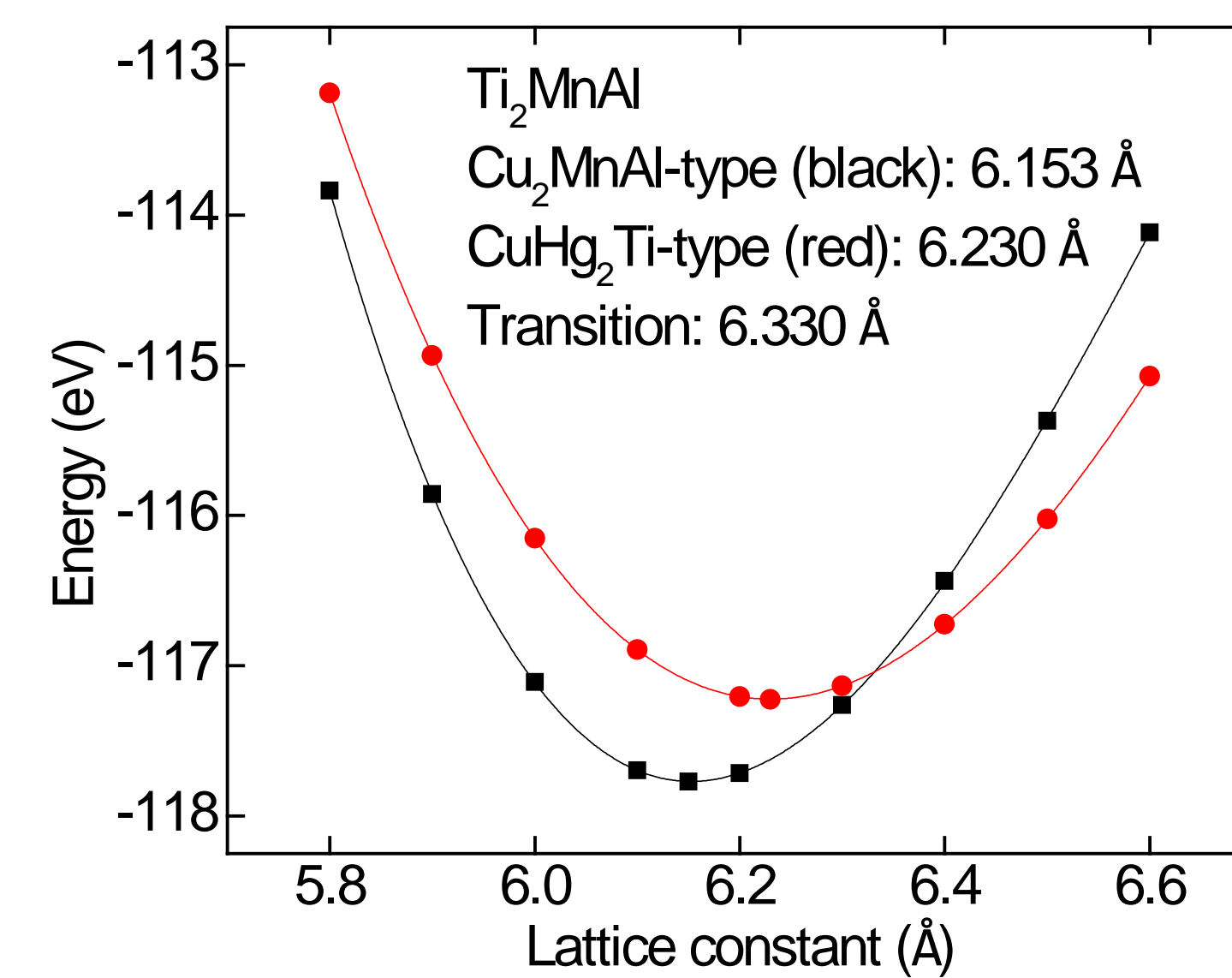
Crystal structure of Heusler alloys



Computational methods

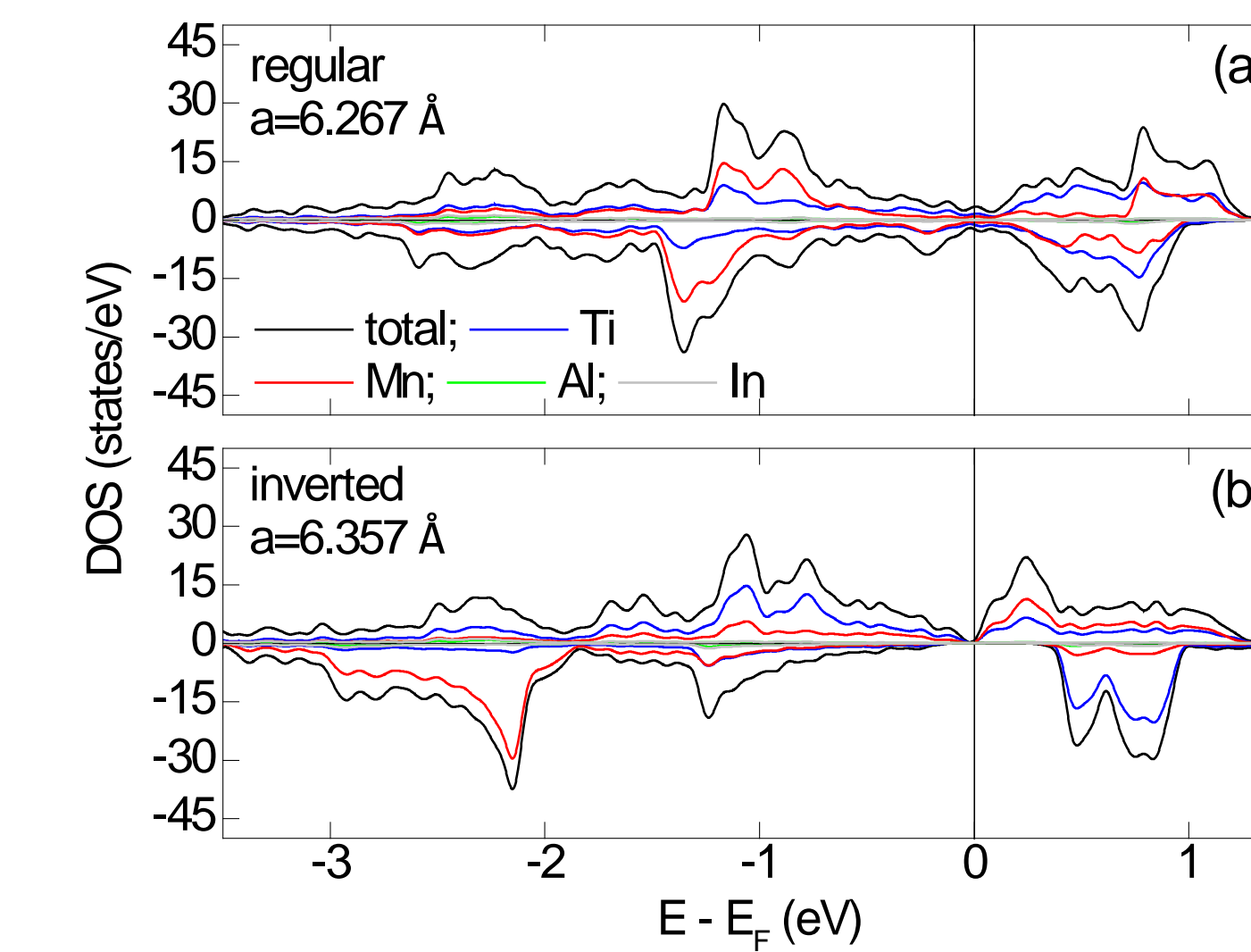
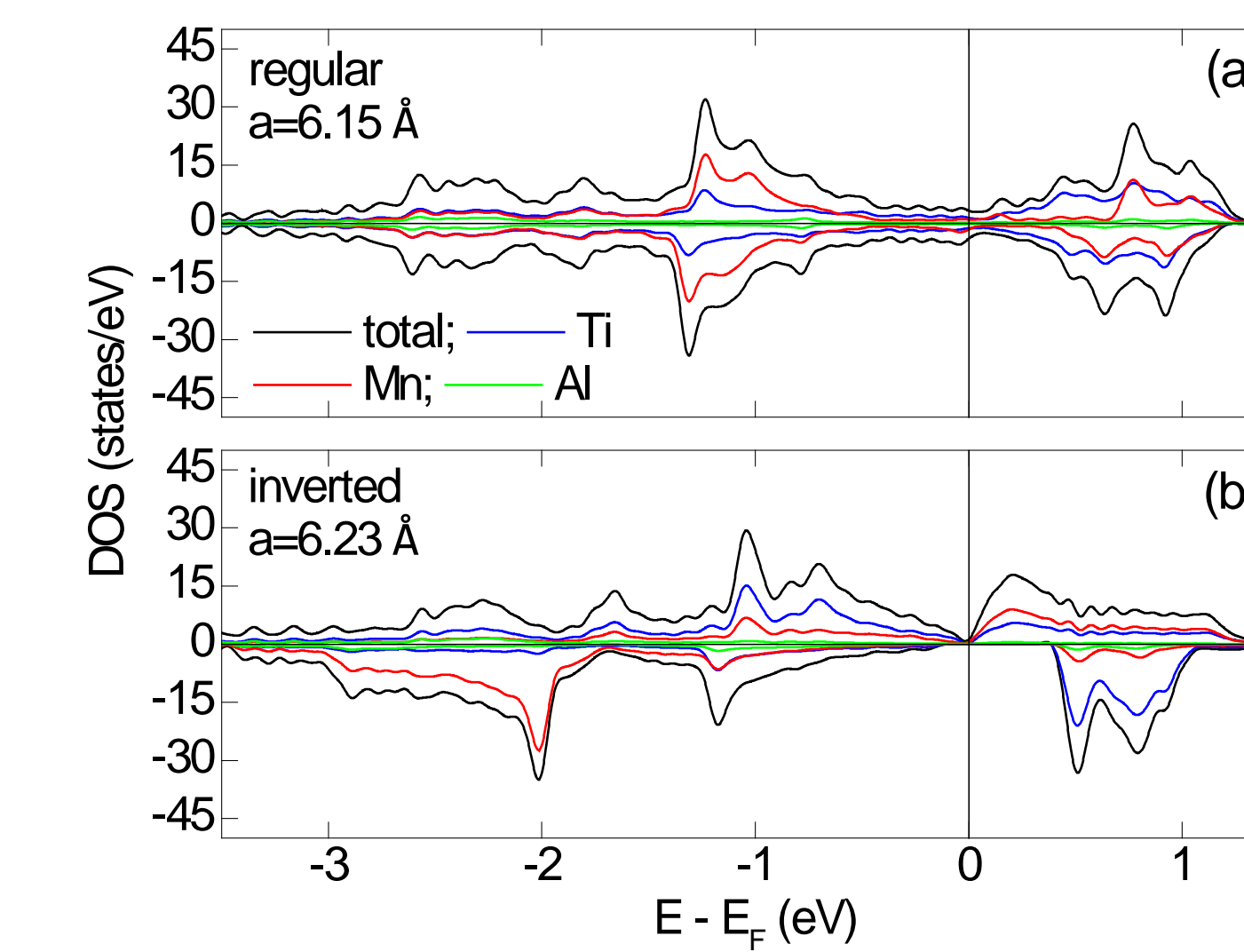
- ✓ Density functional theory (DFT) calculations.
- ✓ Vienna Ab Initio Simulation Package (VASP).
- ✓ Generalized Gradient Approximation (GGA).
- ✓ Convergence criteria: 10^{-5} eV for ionic relaxations and 10^{-6} eV for total energy calculations.
- ✓ Energy cut-off = 500 eV; k -points: $12 \times 12 \times 12$.
- ✓ Extensive convergence tests.

Energy vs. lattice parameter



- ✓ Ground-state structure, defined as the structure of lowest energy, is the regular structure, but at $a = 6.33 \text{ \AA}$, a phase transition occurs, and for larger lattice constants, inverted structure is energetically more favorable than regular one.
- ✓ The transition occurs at a tensile strain of less than 3%, a significant but experimentally attainable value, for example in a thin-film geometry.
- ✓ This suggests a strategy to design new Ti_2MnAl -based SGS or HM compounds in which the lattice parameters can be tuned by elemental substitutions.
- ✓ Based on this materials-by-design strategy, we performed calculations for Ti_2MnAl where 50% of Al atoms are replaced by elements having larger atomic radii, such as Si, Ga, Ge, In, and Sn.

Electronic structure



- ✓ Inverted ground state of $\text{Ti}_2\text{MnAl}_{0.5}\text{Sn}_{0.5}$ exhibits HM behavior, spin-polarized metal.
- ✓ In the case of $\text{Ti}_2\text{MnAl}_{0.5}\text{In}_{0.5}$, the inverted phase, which corresponds to the ground-state structure, is a spin-gapless semiconductor (SGS).

Conclusions

- ✓ We have investigated a previously unconsidered class of materials-by-design, namely substituted Ti_2MnAl .
- ✓ Our first-principles calculations indicate that $\text{Ti}_2\text{MnAl}_{0.5}\text{Sn}_{0.5}$ and $\text{Ti}_2\text{MnAl}_{0.5}\text{In}_{0.5}$ are half-metallic and spin-gapless semiconducting, respectively.
- ✓ In contrast to the metallic Ti_2MnAl parent compound, which has a regular cubic Heusler structure, the substituted alloys are predicted to crystallize in the inverted cubic Heusler structure.
- ✓ P. Kharel, P. Lukashev, S. Gilbert, B. Staten, N. Hurley, R. Fuglsby, Y. Huh, S. Valloppilly, W. Zhang, K. Yang, R. Skomski, and D. J. Sellmyer, Investigation of spin-gapless semiconductivity and half-metallicity in Ti_2MnAl -based compounds. (submitted)

Acknowledgments

- ✓ We acknowledge financial support from the Dean's Office, College of Humanities, Arts and Sciences, University of Northern Iowa.