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## Spin-gapless semiconductivity and half metallicity in Heusler alloys

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# Spin-gapless semiconductivity and half metallicity in Heusler alloys



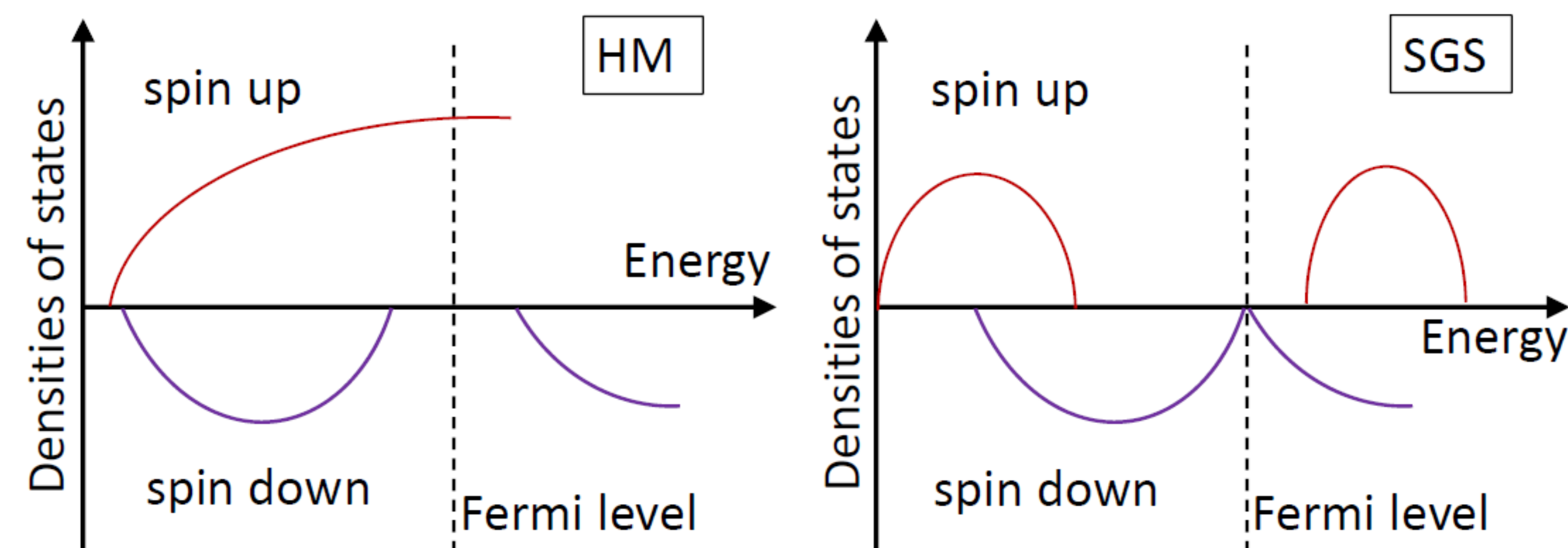
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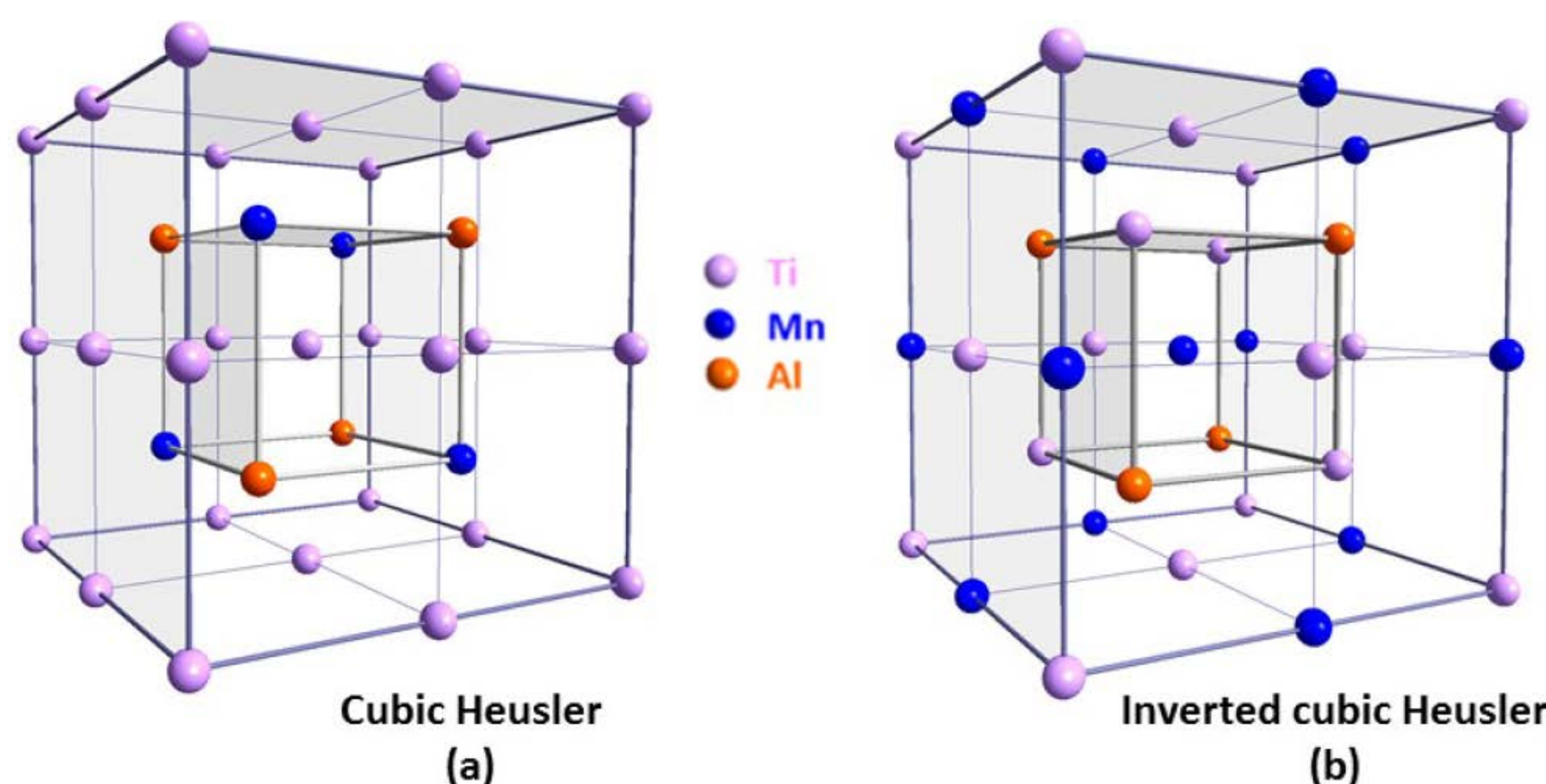


## Motivation and Introduction

- ✓ 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



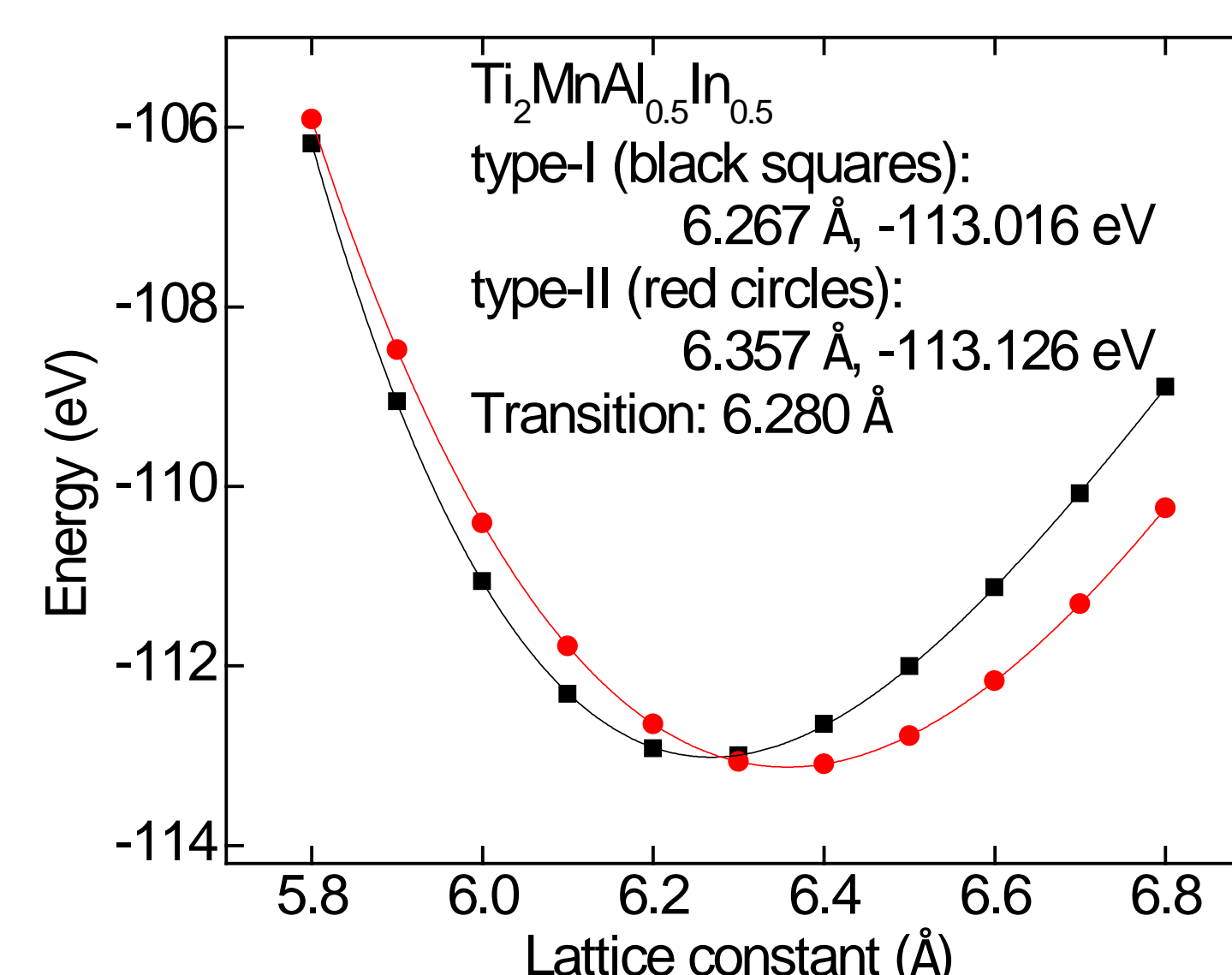
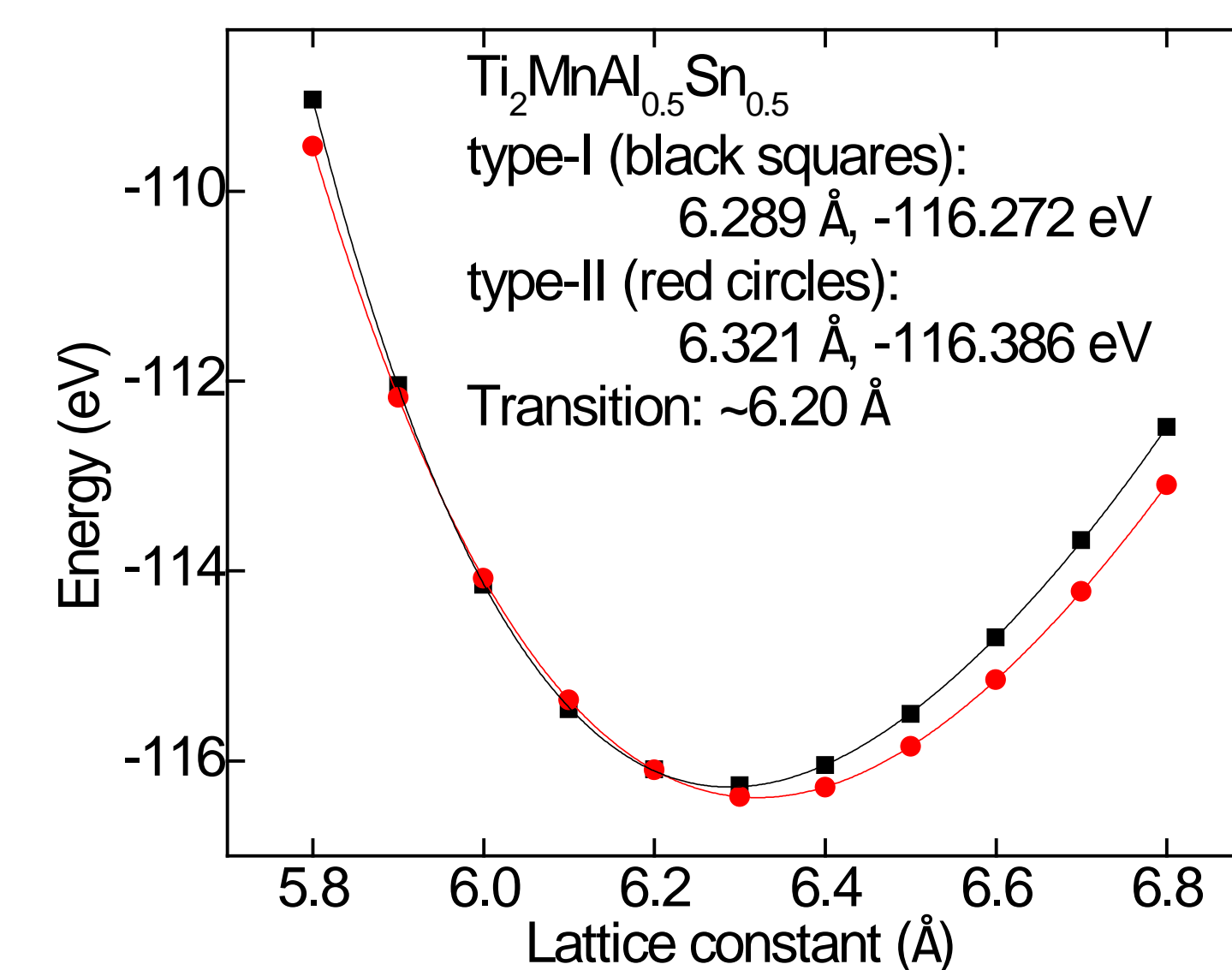
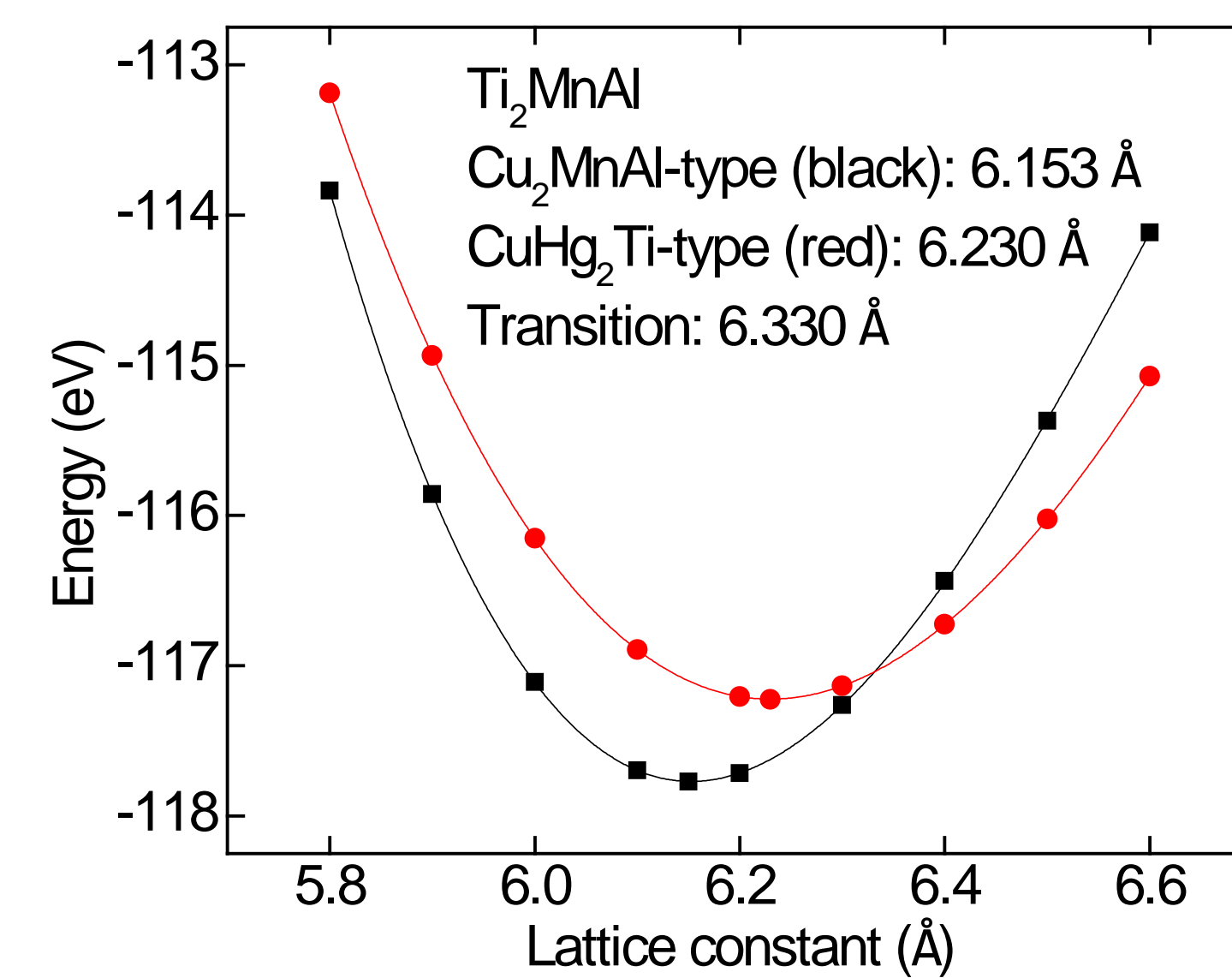
## Crystal structure of Heusler alloys



## Computational methods

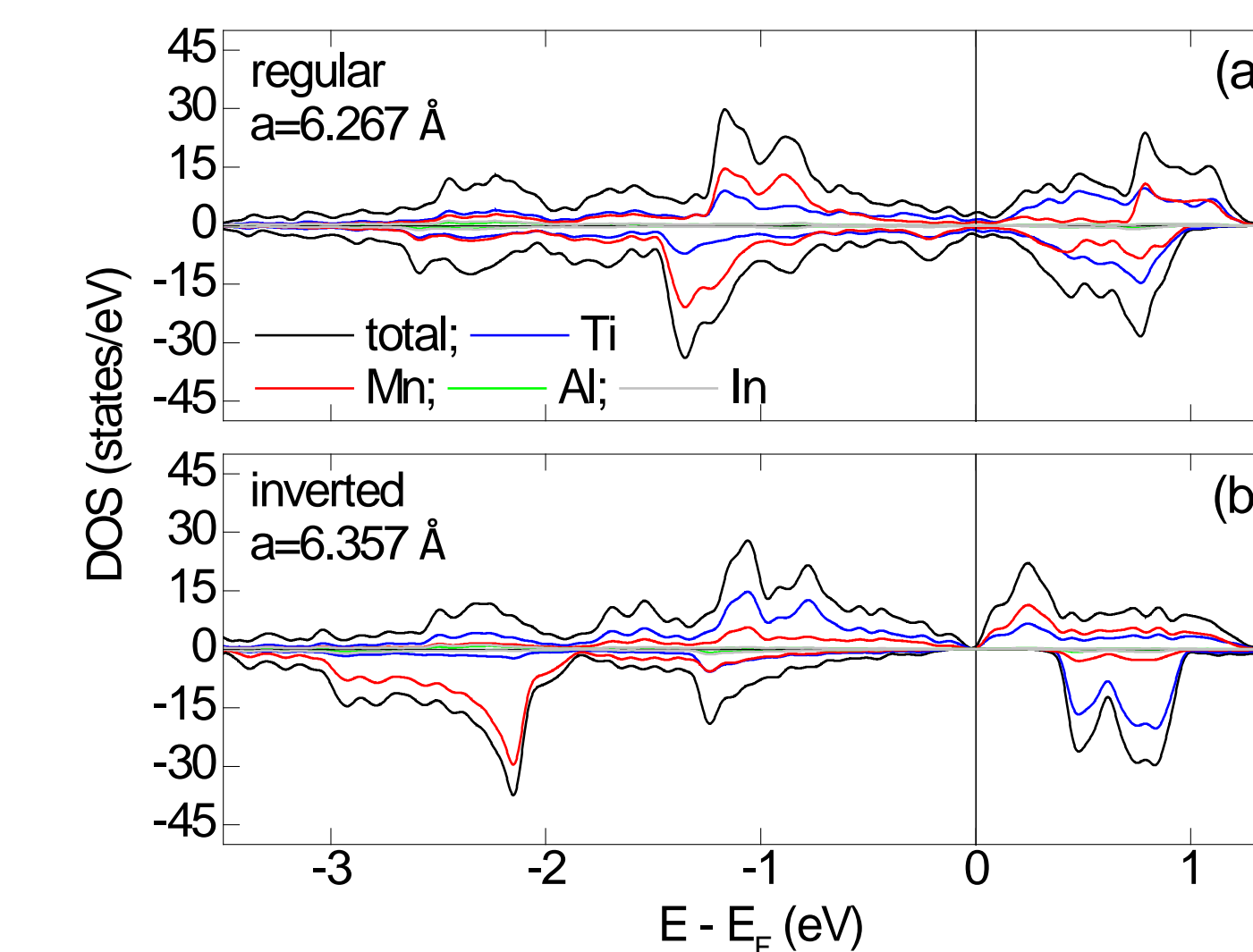
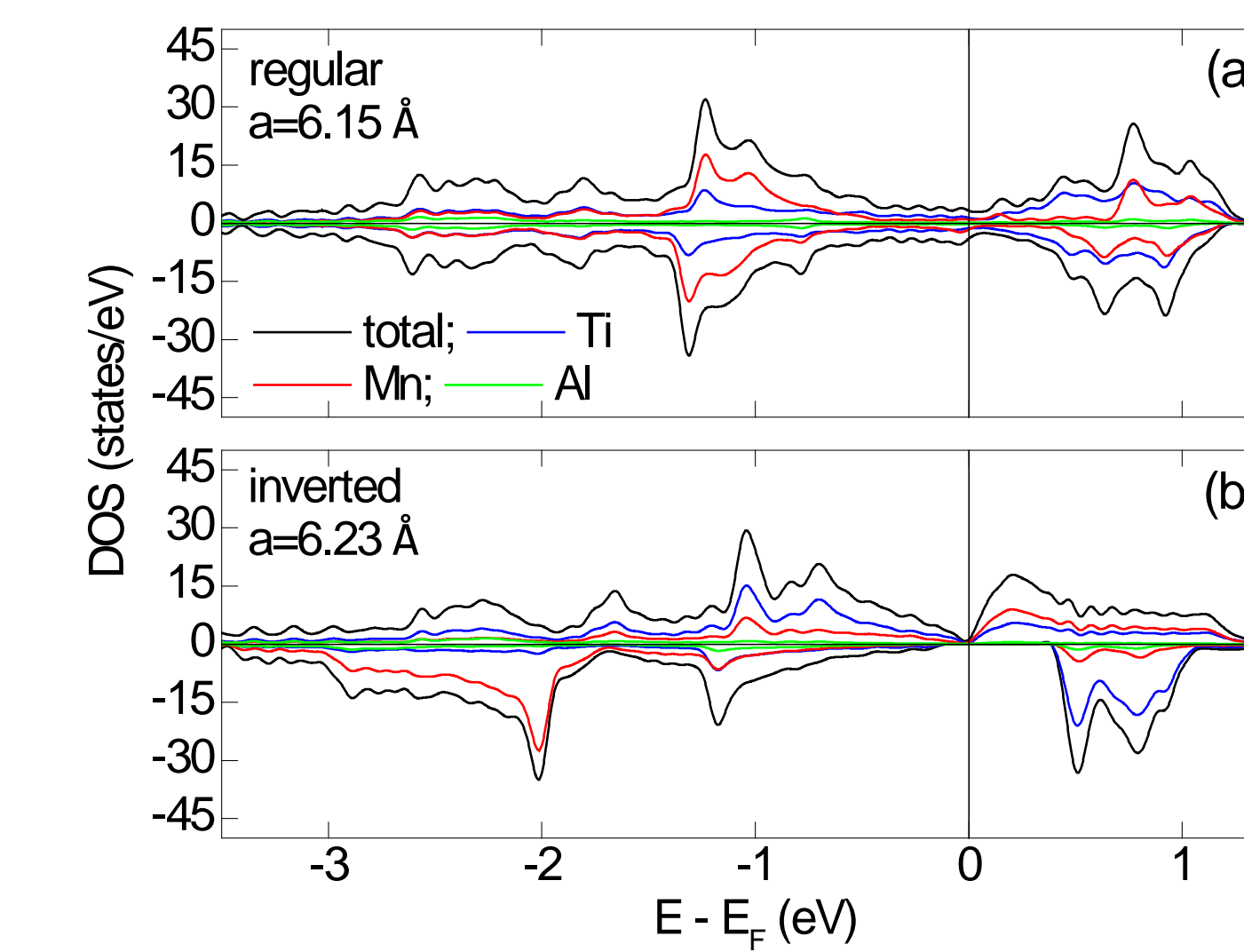
- ✓ Density functional theory (DFT) calculations.
- ✓ Vienna Ab Initio Simulation Package (VASP).
- ✓ Generalized Gradient Approximation (GGA).
- ✓ Convergence criteria:  $10^{-5}$  eV for ionic relaxations and  $10^{-6}$  eV for total energy calculations.
- ✓ Energy cut-off = 500 eV;  $k$ -points:  $12 \times 12 \times 12$ .
- ✓ 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  $\text{Ti}_2\text{MnAl}$ -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  $\text{Ti}_2\text{MnAl}$  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  $\text{Ti}_2\text{MnAl}$ .
- ✓ 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  $\text{Ti}_2\text{MnAl}$  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  $\text{Ti}_2\text{MnAl}$ -based compounds. (submitted)

## Acknowledgments

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