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Spin-gapless semiconductivity and half metallicity in Heusler alloys

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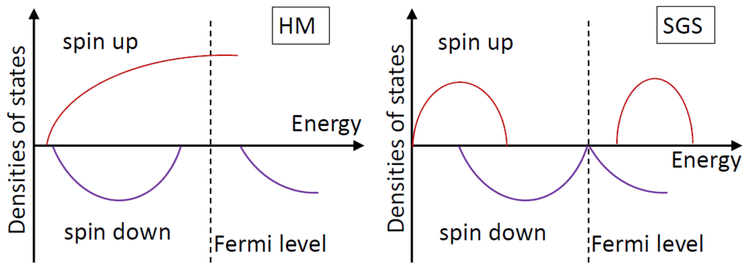
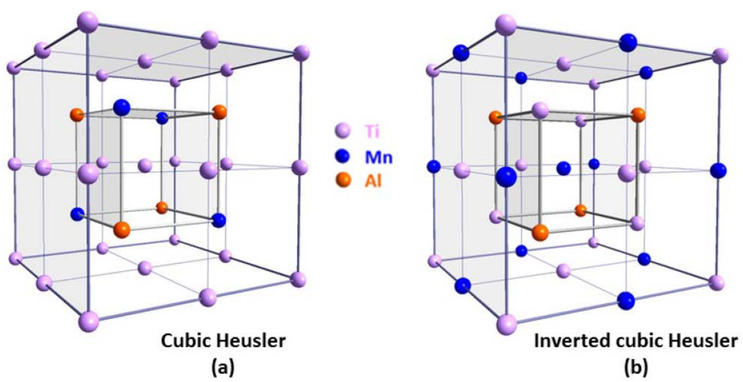
Motivation and Introduction

- ✓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



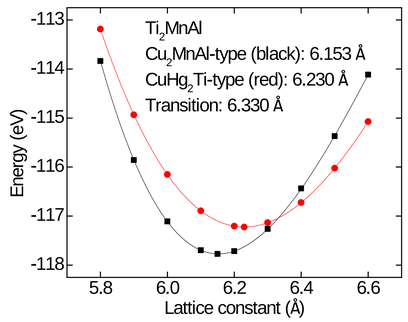
Crystal structure of Heusler alloys

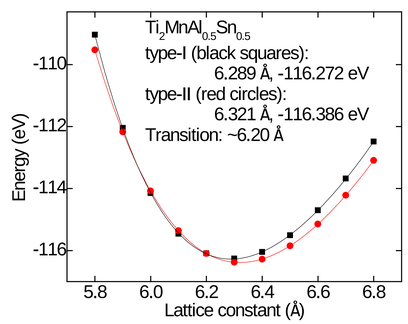


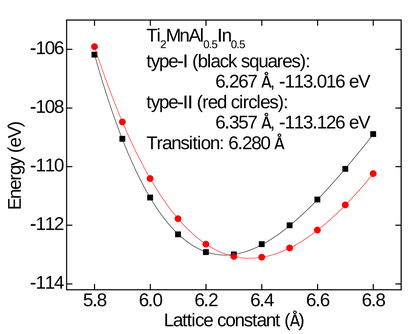
Computational methods

- ✓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: 12x12x12.
- ✓Extensive convergence tests.

Energy vs. lattice parameter

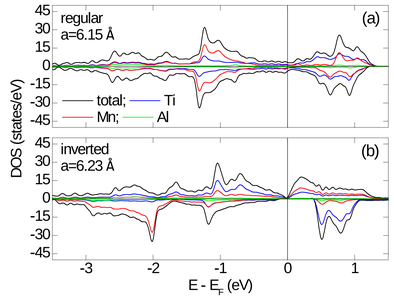




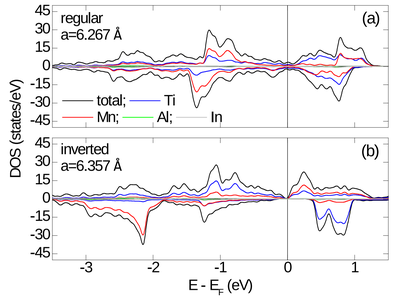


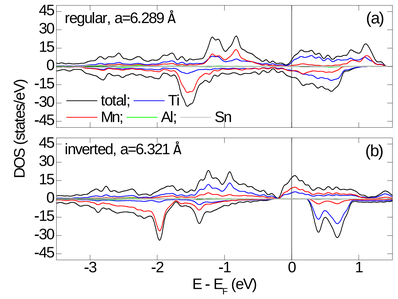
- ✓Ground-state structure, defined as the structure of lowest energy, is the regular structure, but at a = 6.33 Å, a phase transition occurs, and for larger lattice constants, inverted structure is energetically more favorable than regular one.
- ✓The transition occurs at a tensile strain of less than 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 $Ti_2MnAl_{0.5}Sn_{0.5}$ exhibits HM behavior, spin-polarized metal.
- ✓In the case of $Ti_2MnAl_{0.5}In_{0.5}$, 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 $Ti_2MnAl_{0.5}Sn_{0.5}$ and $Ti_2MnAl_{0.5}In_{0.5}$ 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

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