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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, while HM is characterized by complete spin polarization.

Recent investigations have shown that the lattice parameters of Heusler alloys can be tuned by elemental substitutions to transition between HM and SGS.

Computational methods

Density functional theory (DFT) calculations.
Vienna Ab Initio Simulation Package (VASP).
Generalized Gradient Approximation (GGA).
Convergence criteria: 10⁻² 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 Ti₂MnAl-based SGS or HM compounds in which the lattice parameters can be tuned by elemental substitutions.

On this materials-by-design strategy, we performed calculations for Ti₂MnAl where 50% of Al atoms are replaced by elements having larger atomic radii, such as Si, Ga, Ge, In, and Sn.

Conclusions

We have investigated a previously unconsidered class of materials-by-design, namely substituted Ti₂MnAl.

Our first-principles calculations indicate that Ti₂MnAl₀.₅Sn₀.₅ and Ti₂MnAl₀.₅In₀.₅ are half-metallic and spin-gapless semiconducting, respectively.

In contrast to the metallic Ti₂MnAl parent compound, which has a regular cubic Heusler structure, the substituted alloys are predicted to crystallize in the inverted cubic Heusler structure.


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