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HALF METALLICITY AND SPIN GAPLESS FEATURE OF TI_2COSI ALLOY

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Abstract

Half-metals and spin gapless semiconductors (SGSs) with 100 percent spin polarization at the Fermi level are being examined as spintronics candidates. We investigated the impact of uniform strain on the half-metallicity and spin gapless feature of the inverse Heusler Ti2CoSi alloy using first-principles calculations. For Ti_2CoSi, half-metallicity has been observed in the ranges of lattice parameters from 5.874 Å to 6.698 Å for uniform stresses. Ti_2CoSi, on the other hand, is an SGS with lattice constants of 5.852-6.071Å.

Introduction

Spintronics, also known as spin-based electronics, is a fast growing discipline that makes use of both the charge and spin of electrons to develop new breakthrough technologies for next-generation memory storage and computing. The spin injection of highly spin-polarized current from magnetic materials into semiconductors is one of the most important concerns in spintronics. Because the metallic and semiconducting natures coexist in both spin bands, half-metals have 100 percent spin polarisation at the Fermi level. As a result, such half-metals are thought to be promising candidates for spintronics [1]. Inverse Heusler alloys based on Mn_2, Cr_2, V_2, Ti_2, and Sc_2 are likewise half-metals, according to numerous experimental and theoretical studies [2]. Several Ti_2-based inverse Heusler alloys, such as Ti_2Y Al (Y = Mn, Fe, Co, and Ni), Ti_2FeSi, and Ti_2CoSi alloys, have been predicted to be half-metals based on first-principles calculations [3]. Although there have been various investigations on these materials, the effect of strain on half metallicity and the spin gapless feature in inverse Heusler alloys has not been fully investigated. In this context, we used the all-electron full-potential band approach to investigate the effect of strain on the half-metallicity and spin gapless properties of inverse Heusler Ti_2CoSi alloy.

Results and Discussion

It's crucial to look into how strain affects half-metallicity and the spin gapless feature. The case of uniform strain on Ti_2CoSi alloy is investigated in this paper. The total and atom-resolved magnetic moments as a function of the lattice parameter, as well as the conduction band minimum and valence band maximum in the minority-spin band. The equilibrium lattice parameters are represented by solid vertical lines, whereas dotted vertical lines represent a variety of half-metals. In Ti_2CoSi, the minority-spin band gap persists for lattice constants ranging from 5.924 to 6.840Å. Above the lattice parameters 5.941, first-principles calculations revealed that Ti_2CoSi has a half-metallic character, which is compatible with the findings of this work. The energy difference between the valence band maximum and the Fermi level in the minority-spin band, also known as the spin-flip gap (HM gap), is an important quantity for half-metals, as it is the minimum energy required to flip a minority-spin electron of the occupied valence band to the majority-spin Fermi level [4]. The magnetic moments of Ti (A) atoms remain practically constant as the lattice is enlarged, but those of Ti (B) atoms grow dramatically. The magnetic moments of Fe and Co atoms decrease at the same time. The alloys retain their half-metallicity as long as the changes in magnetic moment compensate for each other. The reduced covalent bonding interactions between the transition metals associated with greater atomic distances explain the variations in magnetic moments. Transition metal atoms' spin moments tend to converge with their atomic values. We discovered that the spin gapless property of Ti_2CoSi is only preserved within a narrow range of lattice constants.

Conclusion:

The effects of uniform stresses and tetragonal distortions on the half-metallicity and spin gapless feature of the inverse Heusler Ti_2CoSi alloy were investigated using first principles simulations. The bulk characteristics of Ti_2CoSi alloys match theoretical calculations quite well. The half-metallicity of Ti_2CoSi alloy is more sensitive to tetragonal distortion than uniform strain, according to the findings. Half-metallicity for Ti_2CoSi persists in the ranges of lattice parameters from 5.924 to 6.840 Å for homogeneous stresses. The half-metallic nature of Ti_2CoSi is more susceptible to stresses than the spin gapless characteristic.

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