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Effect of SC Doping on the Electronic Band Structure of $Co_2Ti_{1-x}Sc_xGe$ Heusler Alloy

Preeti Alhan

Department of Physics, Panjab University, Chandigarh-160014, India
*preetibiban92@gmail.com

Abstract

This computational investigation explored the electronic and structural properties of $Co_2Ti_{1-x}Sc_xGe$ Heusler alloys using Density Functional Theory (DFT) within the Quantum ESPRESSO framework. The study employed the Generalized Gradient Approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional, ultrasoft pseudopotentials, and optimized k-point meshes to ensure accuracy in electronic structure calculations. Structural optimization was performed for each Sc doping concentration, allowing precise evaluation of lattice relaxation and defect-induced changes. Spin-polarized calculations revealed the influence of Sc substitution on half-metallicity and spin polarization at the Fermi level, highlighting the tunability of electronic and magnetic properties in these alloys. The results demonstrate that Sc doping modifies the band gap and spin polarization, thereby enhancing the spintronic potential of Co-based Heusler alloys. This work provides a theoretical framework for understanding how substitute defects affect electronic behavior, offering valuable insights into the design of advanced spintronic materials.

Introduction

Heusler alloys have attracted considerable attention in recent years due to their unique electronic and magnetic properties, making them promising candidates for spintronic applications. These intermetallic compounds often exhibit half-metallicity, where one spin channel behaves metallically while the other shows semiconducting behavior, resulting in 100% spin polarization at the Fermi level. Such characteristics are highly desirable for devices like spin valves, magnetic sensors, and quantum computing components [1].

Among the wide family of Heusler alloys, Co-based compounds stand out for their tunable electronic structures and robust magnetic properties. Specifically, Co_2TiGe has been studied for its potential half-metallic behavior and stability. However, the performance of these materials can be further enhanced or modified through doping, which introduces controlled defects and alters the electronic band structure [2].

Scandium (Sc) [3,4] doping in $Co_2Ti_{1-x}Sc_xGe$ provides an effective pathway to investigate how substitutional defects influence the lattice parameters, band gap, and spin polarization. By replacing Ti atoms with Sc at varying concentrations, researchers can explore the relationship between doping levels and electronic properties, thereby identifying optimal compositions for spintronic applications [5,6].

The present study focuses on the effect of Sc doping on the electronic band structure of $Co_2Ti_{1-x}Sc_xGe$. Using Density Functional Theory (DFT) [7,8] calculations, the investigation aims to capture subtle changes in electronic states, band gap variations, and spin polarization. This approach provides a theoretical framework for understanding how doping modifies the half-metallic nature of Heusler alloys, offering insights into their potential for next-generation spintronic devices.

Review of Literature

Mishra, Yadav & Singh (2025) [9] A comprehensive DFT study examined the structural, electronic, magnetic, and thermoelectric properties of Co_2XZ (X = Ti, Hf; Z = Si, Ge, Al) Heusler alloys. The authors confirmed stability in the cubic phase and highlighted the tunability of electronic properties through substitution. Their findings provide a strong foundation for exploring Sc doping in Co_2TiGe, as they establish the baseline electronic behavior of Ti-based Heusler systems.

Mishra & Singh (2023) Investigating Co_2TaZ (Z = Si, Sn) alloys, this DFT study emphasized how electronic and magnetic properties shift under different substitutions. The use of GGA+U improved accuracy in predicting band structures, showing that doping and element replacement significantly alter half-metallicity. This work supports the idea that Sc substitution in Co_2TiGe could similarly tune electronic states and spin polarization.

Jamraoui et al. (2025) [10] A focused study on Co_2FeGe alloys using DFT revealed metallic behavior alongside magnetic character. By analyzing band structures and Fermi surfaces, the authors demonstrated how electronic properties evolve with composition. Their methodology parallels the investigation of Sc doping in Co_2TiGe, reinforcing the importance of substitutional defects in modifying electronic band structures.

Kumar & Gupta (2022) [11] A review on novel Heusler materials for spintronic applications highlighted the multifunctional tunability of these alloys, including half-metallic ferromagnets and spin gapless semiconductors. The authors stressed that substitutional doping is a key strategy for tailoring spintronic properties. This directly aligns with the Sc doping approach, situating Co_2TiGe within broader spintronic material development.

Hirohata & Lloyd (2022) [12] Their review in *MRS Bulletin* emphasized Heusler alloys as ideal spin sources due to half-metallicity at room temperature. They noted that substituting constituent elements can precisely control spin–orbit torque and spin Hall effects. This underscores the relevance of Sc doping in Co_2TiGe, as such substitutions can fine-tune spin polarization and enhance device performance.

Bainsla & Suresh (IIT Bombay) [13] Experimental spin polarization studies on Co_2TiX (X = Ge, Sn) confirmed half-metallic nature and measured spin polarization values around 63–64%. Their work validates theoretical predictions and demonstrates the practical spintronic potential of Co_2TiGe. Building on this, Sc doping can be investigated as a pathway to further enhance spin polarization and band gap control.

Computational Details

The computational study of $Co_2Ti_{1-x}Sc_xGe$ (x = 0, 0.125, 0.25, 0.375) was performed using Density Functional Theory (DFT) as implemented in the *Quantum ESPRESSO* package. Electronic structure calculations employed the Generalized Gradient Approximation (GGA) [14] with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional, which is widely recognized for its reliable description of Heusler alloy properties. Ultrasoft pseudopotentials were used to model ion–electron interactions, while plane-wave basis sets with carefully selected energy cutoffs ensured convergence. Brillouin zone sampling was carried out using a 4×4×4 Monkhorst–Pack k-point mesh, optimized for accurate representation of the electronic density of states and band structure.

Prior to electronic property evaluation, structural optimization was conducted to minimize atomic forces and cell stress below convergence thresholds. For each Sc doping concentration, lattice parameters were relaxed to account for substitutional defects, and the resulting equilibrium structures were used in subsequent analyses. Spin-polarized calculations were then performed to investigate half-metallicity and spin polarization at the Fermi level.This computational framework was designed to capture subtle variations in the band gap induced by Sc substitution, thereby providing theoretical insights into how doping influences the electronic and spintronic potential of Co-based Heusler alloys.

Results and Discussion

The band structure analysis of $Co_2Ti_{1-x}Sc_xGe$ along selected high-symmetry directions in the Brillouin zone demonstrates the impact of Sc substitution on the electronic states of the alloy. In the spin-up channel, the conduction and valence bands remain separated near the Fermi level at lower doping concentrations, thereby maintaining half-metallicity. As the Sc concentration increases, however, the band gap gradually narrows and eventually vanishes, resulting in the loss of half-metallic behavior. In the spin-down channel, additional electronic states begin to intersect the Fermi level with higher levels of Sc substitution, which disrupts the complete spin polarization observed in the undoped compound. The horizontal line at zero energy, representing the Fermi level, clearly illustrates these transitions and highlights the progressive evolution of electronic states as doping concentration increases.

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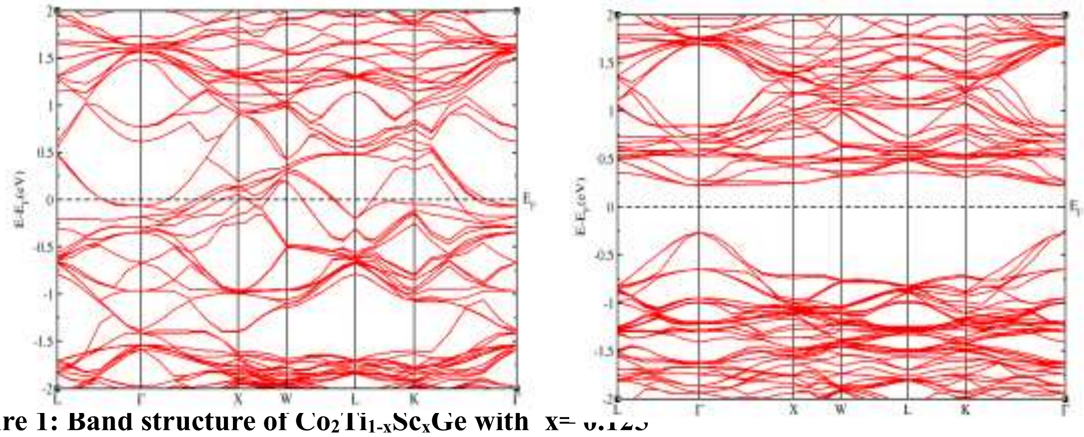

Figure 1: Band structure of $Co_2Ti_{1-x}Sc_xGe$ with x= 0.125

These findings underscore the sensitivity of Co-based Heusler alloys to substitutional doping. At x = 0.125, the alloy continues to exhibit a high level of spin polarization with a band gap of 0.484 eV, yet the introduction of Sc modifies orbital hybridization and shifts the density of states, resulting in a partial reduction of half-metallicity. The observed variations indicate that while small amounts of Sc doping can be accommodated without severely compromising spintronic performance, higher concentrations tend to drive the system toward metallic behavior. This highlights the fine balance between composition and electronic structure, emphasizing that doping levels must be carefully optimized to preserve the desirable spintronic characteristics of Heusler alloys.

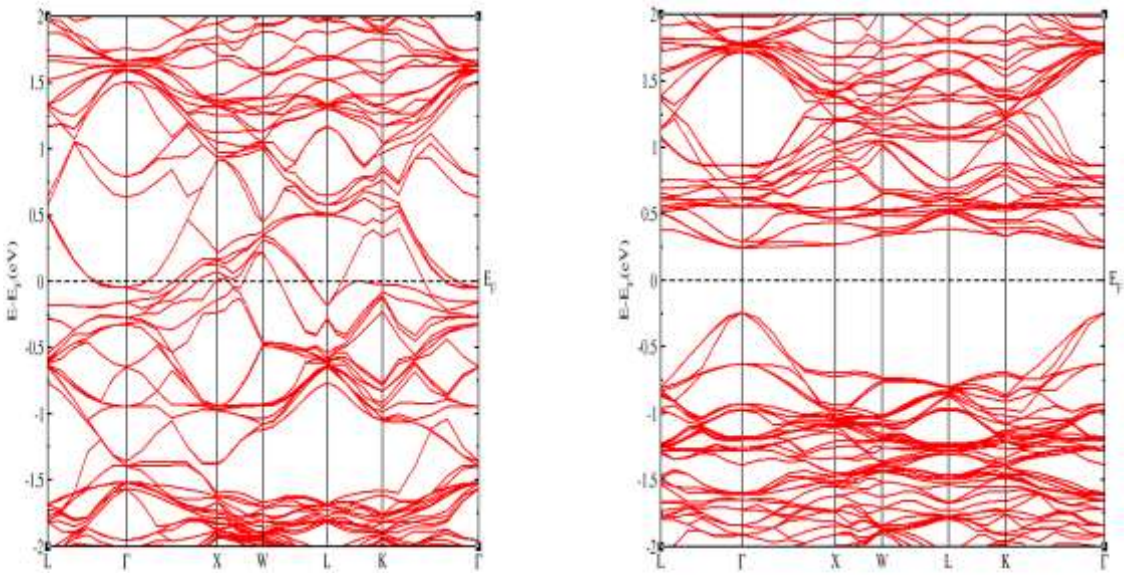

Figure 2: Band structure of $Co_2Ti_{1-x}Sc_xGe$ with x= 0.25

The band structure of $Co_2Ti_{1-x}Sc_xGe$ with x = 0.25, as shown in Figure 6.2, reveals more significant modifications in the electronic states compared to lower doping levels. In the spin-up channel, the band gap becomes narrower, and several conduction bands approach the Fermi level, indicating that the half-metallic nature is beginning to weaken. In the spin-down channel, additional bands intersect the Fermi level, disrupting the complete spin polarization observed in the undoped compound, which originally exhibited a band gap of 0.478 eV. The horizontal line at zero energy, representing the Fermi level, clearly highlights these crossings and confirms that Sc substitution introduces new electronic states, thereby reducing the stability of half-metallicity.

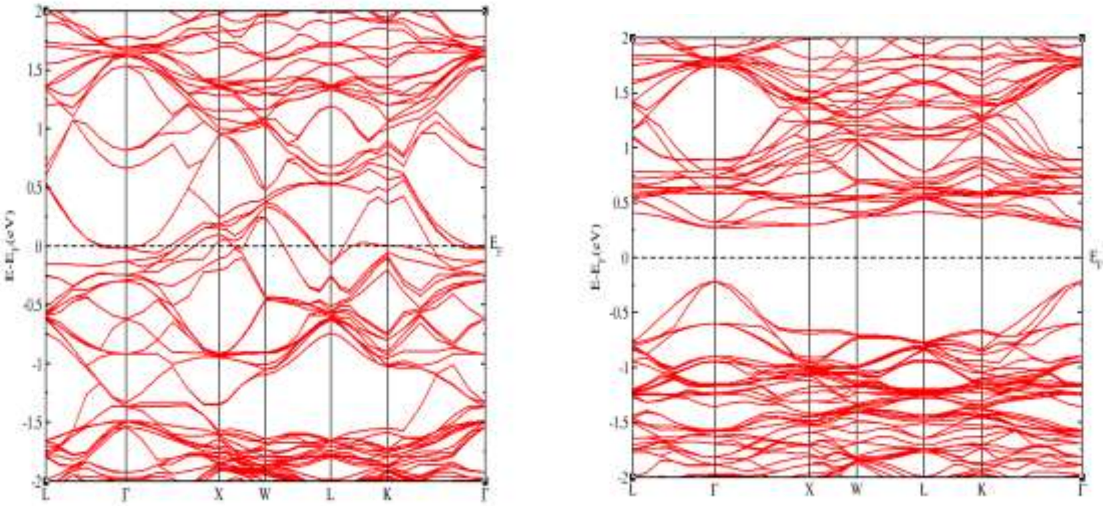

Figure 3: Band structure of $Co_2Ti_{1-x}Sc_xGe$ with x= 0.375

The results indicate that higher levels of Sc substitution significantly modify the orbital hybridization and electronic density of states in Co_2TiGe. At x = 0.375, the alloy continues to exhibit spintronic potential, with spin-up channels contributing to conduction. However, the band structure analysis shows that increasing Sc concentration reduces the band gap, which in turn diminishes spin polarization and weakens half-metallicity.

These observations suggest that while limited Sc doping can be employed to fine-tune electronic properties, excessive substitution destabilizes the electronic structure and compromises the alloy's effectiveness for spintronic applications. This highlights the critical need to carefully regulate defect concentrations and substitution levels in order to maintain the desirable half-metallic character of Co-based Heusler alloys.

Conclusion

The computational study of $Co_2Ti_{1-x}Sc_xGe$ Heusler alloys using Density Functional Theory (DFT) revealed that Sc substitution significantly influences the electronic structure and spin polarization at the Fermi level. Structural optimization ensured accurate modeling of defect-induced lattice changes, while spin-polarized calculations highlighted the potential half-metallic nature of these alloys. The results demonstrate that controlled doping can tune band gaps and magnetic properties, thereby enhancing the spintronic applicability of Co-based Heusler alloys.

Future Implications

These findings provide a theoretical foundation for designing next-generation spintronic materials with tailored electronic and magnetic properties. Future work could extend to experimental validation of Sc-doped Co_2TiGe alloys, exploring synthesis feasibility and stability under real-world conditions. Additionally, advanced computational approaches such as hybrid functionals or GW corrections may refine predictions of band gaps and spin polarization. The insights gained here can guide material engineers in developing efficient, defect-tolerant Heusler alloys for applications in magnetic sensors, spin valves, and quantum computing devices.

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