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Optimizing the thermoelectric behavior of novel quaternary CoIrMnX (X=Sn, Sb) alloys through chemical potential or carrier concentration doping

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ABSTRACT

Materials exhibiting significant polarisation at high spin rates are considered the most promising candidates for spintronic devices. This study investigates the mechanical, optical, spin-polarised electronic structure, magnetism, and thermoelectric properties of CoIrMnX (where X = Sn, Sb). We performed calculations of quaternary Heusler alloys using first-principles calculations. The CoIrMnSn and CoIrMnSb compounds have the most stable Type III crystal structures, according to the calculations performed on the alloys under investigation. We found that the two alloys, CoIrMnSn and CoIrMnSb, possessed a half-metallic ferromagnetic structure, characterised by indirect band gaps of 1.008 eV and 0.806 eV in the predominant spin channels, respectively. Both alloys demonstrate a significant overall magnetic moment of 5 and 6 μβ, respectively. CoIrMnX (where X = Sn, Sb) are ferromagnetic half-metals with 100 percent spin polarisation, according to the results. The results of the elastic constants demonstrate the alloys' mechanical stability. We also investigated optical characteristics such as dielectric function, absorption, reflectance, and optical conductivity. CoIrMnX (where X = Sn and Sb) acts as an efficient absorber in the ultraviolet region and possesses a high refractive index. Alloys exhibit considerable potential as viable candidates for implementation in spintronic devices. The maximum ZT value for CoIrMnSn (CoIrMnSb) is 0.915 (0.6619). To achieve this value, it is necessary to either reduce the charge carrier concentration to $n = 0.0812 \times 10^{20}$ (0.0952×10^{20}) cm^{-3} or the μ to 0.83843 (0.83806) Ryd. Substantially examined materials demonstrate considerable potential for application in the field of thermoelectrics.

1. Introduction

Thermoelectric generators using thermoelectric alloys, which offer sustained power output, have garnered significant interest due to their successful use in spaceship missions over the past two decades. In this study, we aim to investigate the effects of a specific treatment on the participants [1]. The figure of merit, or ZT, calculates the thermoelectric device's energy conversion efficiency based on the Seebeck coefficient S, electrical conductivity σ, absolute temperature T, and the contributions of the lattice k_L and electronic k_e thermal conductivities of the solid materials. These factors are related to each other in the equation: $ZT = \frac{\sigma S^2 T}{(k_L + k_e)}$ [2–4]. Enhancing the power factor, or the figure of merit (ZT), can be accomplished by decreasing the heat conductivity of the material and increasing its electrical conductivity. The achievement of low thermal conductivity (k_L) can be realised by many methods, such as isoelectronic alloying and defect engineering [5–7]. In light of scientific progress and technological advancements, there is a compelling need to develop thermoelectric alloys that possess enhanced electronic and mechanical features. The discovery of a new category of Heusler materials has opened up opportunities for modern technology improvement.

Ternary Heusler (XYZ), full Heusler (X_2YZ), and quaternary Heusler EQH ($XX'YZ$) alloys comprise the majority of Heusler compounds [8]. We produce EQH alloys by substituting an atom of type X′ for one of the X elements in the full Heusler alloys. EQH alloys exhibit comparatively less disorder compared to the ternary Heusler alloy [9]. However, to produce EQH alloys, a lithium ion or another suitable electropositive element fills the appropriate cavities between half Heuslers and full Heuslers, which observe the 24-valence electron rule. They can be easily

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