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# Theoretical perspectives on the electronic, optical, mechanical, magnetic, and anisotropic behaviors of the quaternary Heusler alloys RhFeMnZ and IrMnCrZ (where Z = Si, Ge)

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ABSTRACT

High-spin-polarised materials are the most promising candidates for spintronic devices. Here, the spin-polarised electronic structure, magnetism, mechanical, and optical properties of RhFeMnZ and IrMnCrZ (where Z = Si, Ge) Quaternary Heusler alloys were calculated by first-principles calculations. The calculations show that type III for the RhFeMnSi, RhFeMnGe, and IrMnCrSi and type I for the IrMnCrGe compound configuration is the most stable crystal structure for the studied alloys. The four alloys were found to have a half-metallic ferromagnetic structure with indirect band gaps in the majority spin channels of 0.957, 0.66, 0.745, and 0.891 eV for RhFeMnSi, RhFeMnGe, IrMnCrSi, and IrMnCrGe, respectively. They exhibit an appreciable total magnetic moment of 4 $\mu_B$ for RhFeMnZ (Z = Si, Ge) and 2 $\mu_B$ for IrMnCrZ (Z = Si, Ge). The results show that RhFeMnZ and IrMnCrZ (where Z = Si, Ge) are ferromagnetic half-metals with 100 % spin polarisation. The results of the elastic constants demonstrate the mechanical stability of RhFeMnZ and IrMnCrZ (where Z = Si, Ge) alloys. Optical properties such as dielectric function, absorption, reflectance, optical conductivity, and other optical properties were also probed. In the ultraviolet region, RhFeMnZ and IrMnCrZ (where Z = Si, Ge) are effective absorbers and have a high refractive index. Alloys are promising candidates for potential applications in spintronic devices.

## 1. Introduction

The scientific community has shown increasing interest in the study of Heusler alloys since the theoretical discovery of the first half-metallic (HM) NiMnSb alloy by de-Groot in 1983 [1]. These materials are utilized in spintronics and magnetoelectronics applications [2–8], due to their unique and intriguing structural and magnetic properties. Electrons in one spin channel of these materials demonstrate metallic behavior, while in the other spin channel they exhibit either semiconducting or insulating behavior. The spin polarization is 100 %, and the electronic structure can be adjusted. These materials also have a high Curie temperature [9–11].

Multiple empirical and theoretical research have shown that the quaternary Heusler alloys (EQH) CoFeMnSi alloy has a semi-metallic characteristic [12]. Gao *et al.* [13] established theoretical predictions stating that the EQH alloys CoFeCrAl and CoFeCrSi display complete semi-metallic properties, while CoFeCrGa and CoFeCrGe exhibit almost semi-metallic qualities. In their research, Berri *et al.* [14] studied the electronic and magnetic properties of the CoFeTiSb alloy, known as EQH. They made a prediction that this alloy exhibits a ferromagnetic semi-metallic behavior. Gao *et al.* and Wang *et al.* [15,16] conducted research on Zr-based EQH alloys. Through the use of first principles, they discovered that these alloys are spin-gap-free semiconductors. Moreover, they concluded that Zr-based EQH alloys hold significant potential for applications in spintronics. In their study, Wang *et al.* [17] conducted a thorough analysis of the impact of uniform deformation on the semi-metallic characteristics of FeMnCrZ quaternary HeuslerGG alloys, where Z represents elements such as P, As, Sb, Bi, Se, and Te. In their experimental investigation, Jin *et al.* [18] examined the cubic phase of CoFeCrSi and CoFeCrGe and found that CoFeCrSi exhibits high thermal stability, but CoFeCrGe undergoes disintegration into new compounds at a temperature of 675 K. Bainsla *et al.* [19] experimentally determined that the Curie temperature of CoFeMnGe is around 750 K, and no additional phase transformation occurs up to the melting point. Furthermore, the spin polarization value of 0.67 ± 0.02 in CoFeCrAl is determined using point-contact Andreev reaction measurements [20].

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