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Electronic, Magnetic, and Elastic Features of Quaternary Heusler Alloys: FeVScSb and FeVYSb

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This study employs density functional theory to investigate the structural, elastic, electronic, and magnetic properties of FeVScSb and FeVYSb Heusler compounds. FeVScSb exhibits ferromagnetic properties in its stable state, whereas FeVYSb displays ferrimagnetic behavior. The obtained elastic constants (C_{ij}) indicate that FeVScSb and FeVYSb possess mechanical stability and ductility, while also displaying a significant degree of elastic anisotropy. The aggregate magnetic moment of said alloys is determined to be equivalent to 3 μ_B, in accordance with the Slater–Pauling principle. The investigation of the impact of uniform strain on electronic and magnetic characteristics is conducted. The findings indicate that FeVScSb and FeVYSb exhibit semiconductivity within extensive lattice parameter intervals, ranging from 5.84 to 6.60 Å for FeVScSb and from 6.11 to 6.70 Å for FeVYSb. The Heusler compounds FeVScSb and FeVYSb exhibit half-metallic behavior within a range of lattice parameters. Specifically, FeVScSb displays this behavior when the lattice parameter varies from 6.61 to 6.72 Å, while FeVYSb exhibits half-metallicity within the range of 6.71–6.81 Å. Under the influence of strain, the magnetic moment retains a constant value of 3 μ_B. Therefore, the potential for spintronics is promising.

1. Introduction

The field of spintronics is currently a leading area of investigation in the realm of novel materials exhibiting unconventional properties, which can be attributed to the rapid advancement of nanoscience.[1] The potential of utilizing high-spin-polarization materials in the field of spintronics has generated significant attention among researchers.[2,3] Heusler compounds have been extensively researched due to their high Curie temperature, 100% spin polarization, and tunable electronic characteristics.[4–7] Heusler alloys can be classified into two distinct categories, namely, half-Heusler and full-Heusler compounds. The chemical entities denoted as X, X′, Y, and Z belong to the categories of transition metals and main group members, respectively. The chemical formulas associated with these entities are XYZ, X2YZ, and XX′YZ. Each of the aforementioned chemical formulas exhibits X with a greater valence than X′, and X′ with a greater valence than Y. In 1983, de Groot et al.[8] conducted a study which first proposed that the NiMnSb half-Heusler alloy could exhibit half-metallicity. Since then, electronic structure simulations have revealed that many half-Heuslers with a $C1_b$ configuration and full-Heuslers with an $L2_1$ configuration exhibit half-metallic behavior.[9–13] Several publications[14–17] have shed light on the rule of Slater and Pauling, which establishes a connection between the electronic and magnetic features, and the process by which the gap in Heusler alloy is formed. In addition, ternary Heusler alloys (NiMnSb, Co_2CrAl, CoMnGe, and Ni_2MnGa) have been extensively examined[18–22] for the impact of lattice distortions on magnetic and electronic characteristics.

A recent hypothesis posited that compounds of the LiMgPdSn type may demonstrate characteristics of half-metallicity, as indicated by sources.[23,24] The Y-type solids are characterized by the space group $F\bar{4}3m$. The CoFeMnSi compound serves as a prototypical model and has been the subject of extensive investigation by numerous research groups.[25–27] Dai et al.[24] inferred that CoFeMnSi is likely to exhibit a half-metallic property based on the analysis of its XRD pattern and magnetic measurements. The crystal structure of CoFeMnSi was found to be similar to that of LiMgPdSb. The hypothesis that CoFeMnSi exhibits a half-metallic property has been corroborated by both experimental

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