INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

Experimental synthesis and theoretical prediction of half-metals in Heusler family have been the driving force in searching new materials for spintronics applications. In order to understand the physics of half-metals in a systematic way and without being material specific, in this thesis, we have explored in details 54 ternary compounds (six ternary series)$X_2X'Z$ and 36 quaternary compounds (four quaternary series) CoX'Y'Z as the daughter compounds of these ternary compounds, where X = Mn, Fe, Co; X' = 4d transition metal atoms across the 4d row of the periodic table; Y' = Mn, Fe and Z= Al, Si. The major motivation for this work was to explore the compounds across several series by changing one or two of the constituents to get insights into the roles of the different magnetic constituents along with that of the main group elements. A comprehensive overview of these compounds, addressing the trends in structural, electronic, magnetic properties and Curie temperature has been presented here along with the search for new half-metals. A simple picture of hybridization of the d orbitals of the neighboring atoms is used to explain the origin of the half-metallic gap in these compounds. We have shown that the arrangements of the magnetic atoms in different Heusler lattices are largely responsible for the interatomic exchange interactions that are correlated with the features in their electronic structures as well as with the possibility of occurrence of half-metallicity. To find out the role of 4d elements in these properties we have made one to one comparison between the isoelectronic pair of ternary (quaternary) compounds where in one case the magnetic constituents are all 3d transition metal atoms and in the other one of them is a 4d transition metal atom. We found that the major features in the electronic structures remain intact if a 3d X' constituent is replaced with an isoelectronic 4d element as long as the crystal structure of the pair of compounds are same, implying that the total number of valence electrons can be used as a predictor of half-metallic nature in compounds from Heusler family. We have also explored the phenomenon of site-dependent substitution affecting half-metallic behavior and the possibility of half-metallic behavior in chemically disordered Heusler compounds. In a nutshell, the results presented in this thesis provide important insights into the evolution of half-metallicity in Heusler compounds.