



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI  
SHORT ABSTRACT OF THESIS

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Thesis Title: **First principles study of phase stability, electronic structure and magnetism in Mn<sub>2</sub>YZ systems with multiple functionalities**

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**SHORT ABSTRACT**

Heusler compounds are a remarkable class of intermetallics which possess many functionalities including magnetic shape memory effect (MSME), half-metallicity, magnetocaloric effect and magnetoresistance with many possible applications. In the family of Heusler compounds, Mn<sub>2</sub>YZ compounds have attracted considerable attention due to their interesting structure-magnetism relations leading to applications in magnetomechanical devices, magnetic sensors, spintronics, and energy technology. In this thesis, we investigate the phase stability, structural, electronic, elastic and magnetic properties of several Mn<sub>2</sub>YZ systems from first-principles electronic structure calculations. The primary motivation is to explore and understand the possibility of martensitic phase transformation leading to magnetic shape memory effect and its origin in several pristine and substituted Mn<sub>2</sub>YZ systems. In this thesis we investigate Mn<sub>2</sub>NiGa, Fe and Co substituted Mn<sub>2</sub>NiGa, Mn<sub>2</sub>FeGa and Mn<sub>2</sub>Ni<sub>1+x</sub>Sn<sub>1-x</sub> compounds. The choice of the systems is motivated by the interesting experimental results obtained in each case. A complete picture of martensitic phases and the path of phase transformation in magnetic shape memory alloy Mn<sub>2</sub>NiGa is explained from the electronic structure, phonon dispersion, and electronic susceptibility. The effect of Fe and Co substitution on the martensitic phase transformation, mechanical stability, magnetization and the magnetic ordering temperature of Mn<sub>2</sub>NiGa is investigated extensively, leading to establishing several important differences in physical properties with well known magnetic shape memory system Ni<sub>2</sub>MnGa. The origin of different structural phases and complex magnetic orders resulting out of it in Mn<sub>2</sub>FeGa is investigated leading to the knowledge of the ground state spin structures in each structural phase which was hitherto unknown. Finally, the effect of compositional changes along with different atomic and magnetic ordering on martensitic transformations is investigated for Ni-excess, Sn-deficient Mn<sub>2</sub>NiSn which have experimentally observed to exhibit magnetic shape memory effect. In a nutshell, the results presented in this thesis provide us with significant insights into the fundamentals of Mn<sub>2</sub>YZ systems and demonstrate how functionalities can be manipulated in these systems by changing compositions and/or by substitution.