



# Full Heusler alloys (Co<sub>2</sub>TaSi and Co<sub>2</sub>TaGe) as potential spintronic materials with tunable band profiles



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## ABSTRACT

DFT based structural optimizations and cohesive energies of novel Co-based Heusler compounds confirm the stability of these alloys in L<sub>21</sub> phase (Cu<sub>2</sub>MnAl prototype). Later, the equilibrium lattice constants are predicted. While defining the electronic structure, the modified Becke Johnson scheme for exchange correlations predicted more efficient results than the generalized gradient approximation and onsite Hubbard approximation. Calculated band structure and densities of states together with spin magnetic moments designate the half-metallic character of these alloys. The elastic constants are calculated to define the mechanical stability and ductile nature of these alloys. The ferromagnetic spin moments amount to an integral value of 3μ<sub>B</sub> for each system with a maximum contribution from transition metal cobalt atom. Present study opens a way out for the potential application of these alloys as spintronic materials.

## 1. Introduction

Heusler systems have grabbed lot of attention due to their peculiar properties like high spin polarization, interesting electronic structure (half-metallic/semiconducting/spin gapless nature), shape-memory effect, large Curie temperatures, ferromagnetism and thermoelectric properties, which are used in various applications like magnetoresistive materials, spin valve generators, spin filters, transducers, shape memory devices and spintronics [1–4]. Among them half metallic ferromagnetic (HMF) materials are a class of materials that have been acknowledged by the world class researchers due to their application in spintronics/magneto electronics/thermoelectrics [5,6]. Thus, spin-based electronics are expected to bring revolution in the field of information technology, memory devices and telecommunication. The addition of the spin degrees of freedom to the conventional electronic devices has several advantages like non-volatility, increased data processing speed and decreased electrical power consumption. In these materials spin resolved bands have special behavior, the majority spin band shows metallic character while the minority spin band shows semiconducting/insulating behavior with a gap at Fermi level. The HMF exhibit 100% spin polarization at Fermi level which is supposed to increase efficiency of spintronic devices [7,8].

Besides being used for spintronic applications Heusler alloys have also been studied for thermoelectric applications [9]. The materials with high thermoelectric coefficients have been a subject of interest to researchers worldwide as they effectively convert waste heat into electrical energy [10]. The efficiency of thermoelectric material is given by dimensionless figure of merit ( $zT$ ) given as  $zT = S^2 \sigma T / \kappa$ , where  $S$  is power factor,  $\sigma$  is electrical conductivity,  $\kappa$  is thermal conductivity and  $T$  is temperature. The efficiency of thermoelectric materials can be increased by increasing  $zT$  which can be done by maximizing Seebeck coefficient, electrical conductivity and minimizing thermal conductivity [11,12].

Various Co<sub>2</sub> based Heusler alloys like Co<sub>2</sub>MnBi, Co<sub>2</sub>FeAl, Co<sub>2</sub>FeAl, Co<sub>2</sub>FeAl and Co<sub>2</sub>MnSi [13–15] have been investigated for their half-metallic, transport, magnetic properties so far. Lately, full Heusler alloys Co<sub>2</sub>TaX (X = Al, Ga, In) have been predicted to be half-metallic ferromagnets with high Curie temperatures [16]. Earlier to this, Co<sub>2</sub>TaAl was experimentally reported to be a ferromagnetic half-metal with lattice constant equal to 5.9 Å [17]. In this study, we have considered the magneto-electronic, elastic and thermoelectric properties of new full Heusler compounds; Co<sub>2</sub>TaSi and Co<sub>2</sub>TaGe. Our calculations are the first ever intuitions on such material properties which are discussed in following subsections.

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