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First Principles Calculations on the Electronic, Elastic, Structural, and Magnetic Properties of Co_2RuGe and Co_2NiGe FH Alloys

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ABSTRACT

Utilizing first principles, the structural, elastic, magnetic, and electronic properties of Co_2YGe FH (Full-Heusler) alloys where Y is Ni, Ru have been examined. The partial and total densities of states, as well as electronic band structures, have been calculated. The Co_2YGe alloys half metallic-nature is confirmed by the computed band structures, which show that the valence and conduction bands in the up spin channel overlap at the Fermi-level while here is a band-gap between them in the down spin channel. These compounds have ½ (half) metallic properties, as seen by the TDOS and PDOS. According to mechanical characteristics, the alloys Co_2NiGe and Co_2RuGe are highly stiff and they respectively are ductile and brittle. By their magnetic characteristics this is demonstrated that compound have Para magnetism property as their net magnetic moment is not zero. According to the results, these alloys could be a contender for spintronic devices.

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1. Introduction

Recently HM compounds have attracted a lot of devotion from investigator's and researchers due of their multiple spintronic uses, (Du et al., 2021; Shakil et al., 2021). The IT (information technology), telecommunications, and memory devices have all been transformed by spintronic technologies. The data dispensation capabilities and low power consumption of the aforementioned devices have been improved by their wide-ranging usage of HM Heusler alloys (HA) (Nagura, Ashani, Adebambo, Ayedun, & Adebayo, 2021; Uğur et al., 2021). Due to their distinctive characteristics, including SP (high specific surface area), and high Curie temperature (Tc), half metallicity, shape memory effect, thermoelectric capabilities, and ferromagnetism (Çanlı, Ilhan, & Arıkan, 2021; Govind et al., 2021; Gupta, Sinha, & Verma, 2021; Ullah & Khalid, 2021; Y. Zhang & Xu, 2020), HA have grown to be particularly intriguing materials.

A variety of applications, including shape memory devices, energy technologies, gigantic magneto- resistive materials, transducers, multiferroics, tunnel junctions, and spin filters, magneto-caloric applications, utilize HA because of their noteworthy properties. HA could also be used in thermoelectric in addition to spintronic (Uğur et al., 2021). Investigators are very interested in these materials due to high thermoelectric coefficients values because they are effective at converting excess heat energy into electrical energy. If S and σ were to increase as a function of T (temperature) (Essaoud & Jbara, 2021), the efficacy of these molecules might be boosted. In this concern, numerous recent studies on these materials have been conducted, as stated in the literature Fritz Heusler found the first HA (Cu2MnAl) in 1903, and define the fact that its component parts are not of different FM

(Tariq, Mubarak, & Hamioud, 2021), it displayed FM behavior. HA are primarily divided into two categories: half HA and FH alloys. The composition of half of HA is given by the formula XYZ (Hadji, Khalfoun, Rached, & Azzouz-Rached, 2021), where Y and X are transition metals (TM) and member of the key group of elements is represented by Z (Hao, Liu, Fan, & Wang, 2020). Due to the involvement of three different types of elements in half and full HA, these materials constitute intermetallic ternary- compounds (Idrissi et al., 2019).

Among all HA kinds, FH alloys have garnered the most interest due to its application in spintronic application because of the 100% SP presence of HM character. De Groot and his coworkers were the first one whose identified the half metallicity of NiMnSb HA (Fan et al., 2020). Different Spin-channels have diverse spin orientations for all HM materials, with metallic properties for one spin direction and insulating or semi-conducting characteristics for the further (Arnold et al., 2016). Co-based FH alloys are of particular concern since they exhibit favorable magnetic characteristics and have high MM and Tc. Cobalt (Co) based alloys exhibit HM property, even at room temperature according to earlier theoretical predictions (Ghosh et al., 2019). Many substances have been studied in the past. In this description, the electrical, magnetic, elastic, and structural properties of a novel class of FH (full Heusler) alloys, Co_2YGe(Y=Ni, Ru), are studied because there is still a growing market for these materials. The proposed alloys' HM nature is indicated by the DFT technique used to finish the current work. These compounds can be extremely important in spintronic devices because they are entirely spin polarized.

2. Computational Method

In order to calculate the physical parameters of Co_2YGe(Y=Ni, Ru), the FP-LAPW scheme was used in conjunction with the WIEN2k coad and the DFT technique (Ilkhani, Boochani, Amiri, Asshabi, & Rai, 2020). All the attributes were calculated using the GGA-PBE functional. In addition to GGA method was used to calculate the band structure and DOS of Co_2YGe. The Charpin method is used to derive C44, C12, and C11 are three elastic-constants of cubic system (Rüßmann et al., 2017). The size of the prime vector in a Fourier expansion of charge density is determined by G_{max}. The core separation energy, which separates valence states from core states, was adjusted to -6.0 Ry. During the self-consistent field (SCF) cycle, the charge levels and energy of the convergence criteria were 0.001e and 0.0001Ry. RMT, K_{max} = 8, where RMT is the smallest because circle of muffin-tin span within the unit cell and K_{max} is the largest size of k-vector within the regular lattice, is known as the most exciting reverence circle of the muffin-tin and the item of wave-vector (Sun, Wu, Ali, Felser, & Yan, 2015). According to the chart, the vitality of the ground state and the number of k points are used to determine the number of k-focuses. The fewest k-points that are most closely associated with a steady ground state vitality are used to transport the fundamental limitations of merging. In this way, the 10x10x10 k-mesh that provides the best fit for the materials observed was taken into consideration in order to establish self-consistency inside the first Brillouin Zone (BZ) (Nielsen & Ninomiya, 1983).

3. Results and Discussions

3.1. Structural Properties

The cubic crystal structure of complete-Heusler alloys with the formula Co_2YGe alloys, where Y is Ni or Ru in different alloys, is found in the Fm no. 225 space group. The following table lists Co_2YGe structural characteristics. The cubic structure of Co_2NiGe and Co_2RuGe has atomic positions for Co_2 (3/4,3/4), Ni, Ru (0,0), and Ge(1/2,1/2).

3.1.1. Optimization

Optimization graph identified the overall energy of any system in order to determine right energy of that system. This energy has to finish two processes in order to calm the condition. First, it is established how much force is exerted internally within the primitive cell. Because the u parameter is the smallest at this point and the outcome forces have been minimized. After calculating the c/a numbers, which represent the lattice constant ratio, the total energy of the system is obtained in a subsequent step. Using Brich-Murnaghan equation, the energy curve with respect to volume has been optimized (Xu et

al., 2021). The following diagram illustrates the optimum curve for the chemicals under study.

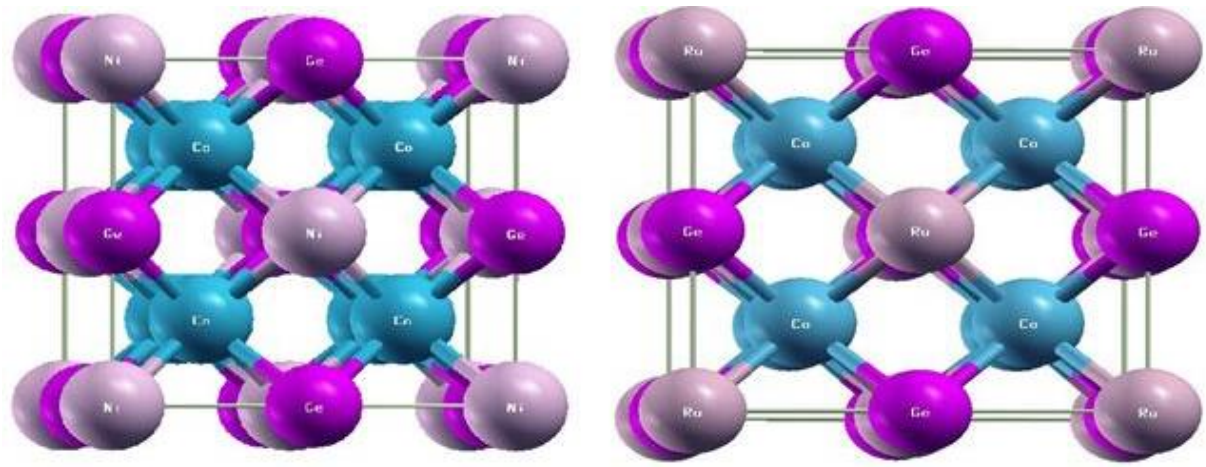

Figure 1: Structure depiction of complete Co_2YGe Heusler alloys

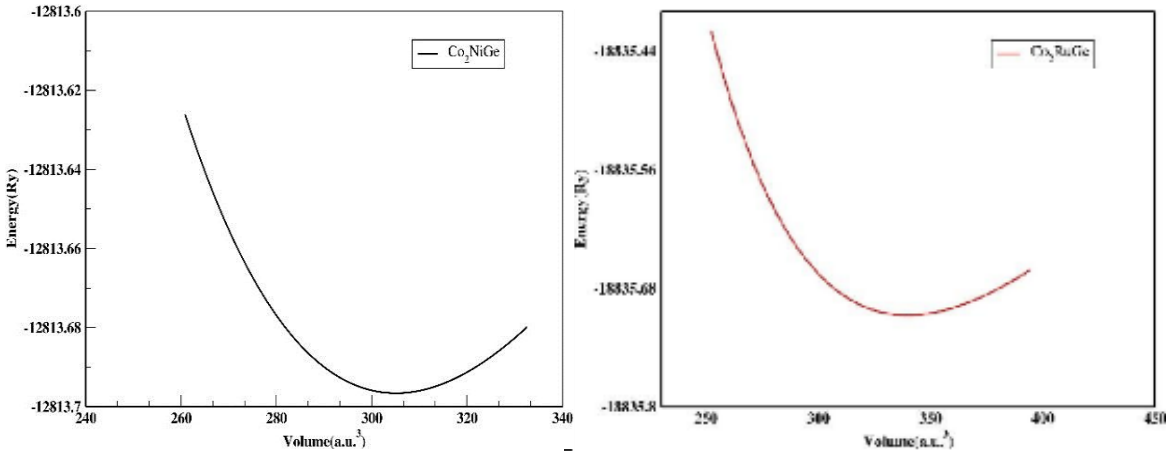

Figure 2: The total energy optimization curve with respect to the volume of Co_2YGe alloys where Y=Ni, or Ru

Table 1
The table below showing the calculated values

Lattice Parameters	Co_2NiGe	Co_2RuGe
a(Å)	5.78	6.09
B′	5.00	4.99
Bo(GPa)	235.92	207.24

3.2. Electronic Properties

3.2.1. Band Structure

By applying the PBE-GGA+U computation, it can define electronic energy range and as well as band structure of electrons inside of an equilibrium point in the first BZ (Brillion Zone) (ZXPN) (Wang, Wu, Shi, & Wang, 2016), figure 3(a, b) illustrate complete description of both compounds by PBE-GGA+U calculations.

According to above pictures description of both compounds exhibit metallic behavior when spin-up Fermi levels are present because this causes the valance band and conduction band to overlap (Bonilla, Téllez, Rodríguez, Aguiar, & Roa-Rojas, 2008). The valance band and conduction band, however, have a small gap in the case of spin-down, which exhibits non-metallic behavior. Overall, both compounds behave in a semi-metallic manner. The Fermi level Ef, which is shown in the accompanying picture as a black dotted line and is located at 0 eV, separates the occupied band from the unoccupied band.

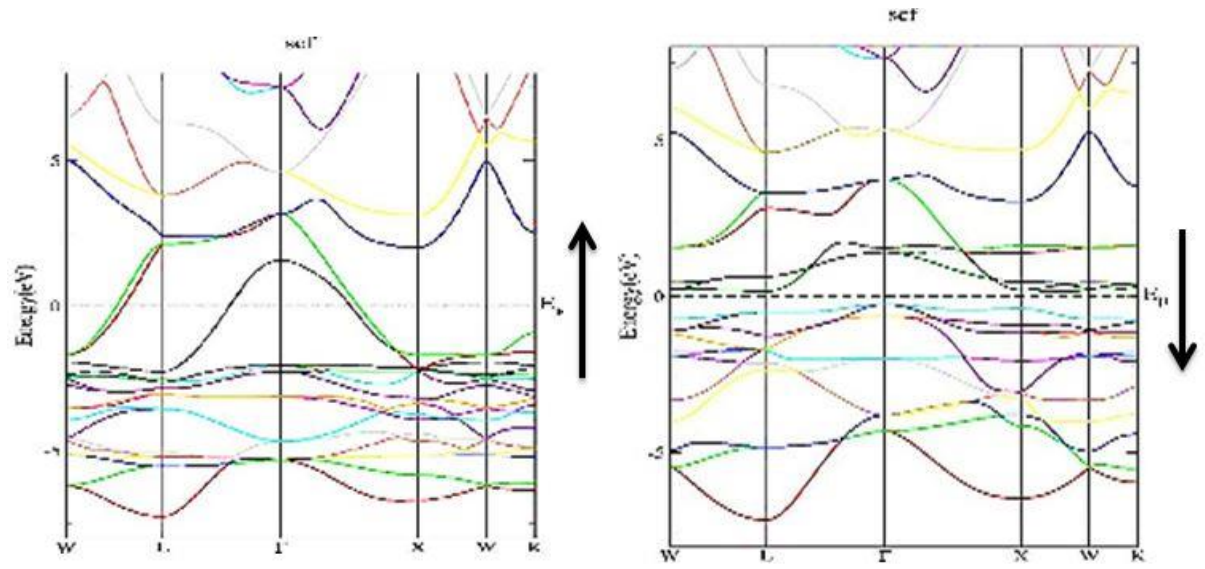

Figure 3(a): Electronic-band structure description of Ni substituted Co_2YGe alloy

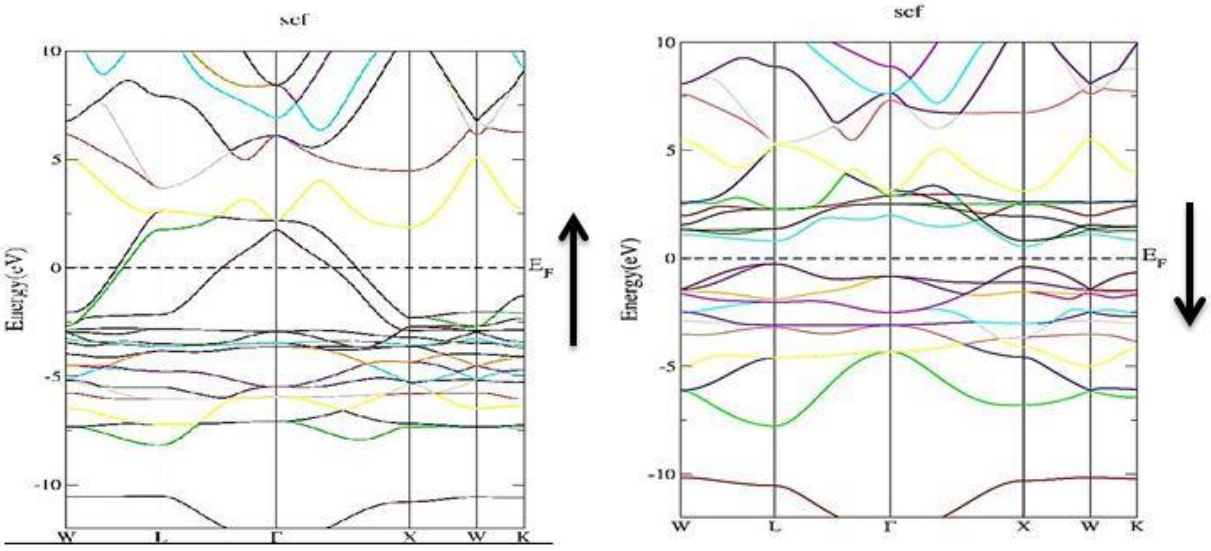

Figure 3(b): This graph illustrate electronic-band structure of Ru substituted of Co_2YGe alloy

3.2.2. Density of States (DOS)

To better understand the electronic characteristics and described the band structures of the compounds, we find the TDOS (total density of states). The DOS is the total number of states that an electron can access in one unit of space at a given energy level (Rahn et al., 2018). Using PBE-GGA+U parameters, we have resolved the TDOS of Co_2NiGe and Co_2RuGe in the range of -8 to 8 eV in the current work. Diagrams show that the TDOS is designed with two bands. The valance band (VB) and conduction band are shown on the left and right sides, respectively, of the fermi level Ef (CB). Describe how the half-metallic behavior of the TDOS is seen in the understudied compounds. In the case of Co_2RuGe and Co_2NiGe respectively, the energy gap between the valance and conduction band is 0.4 eV and 1.3 eV. The contribution in the valence band because of their hybridization process that occurred b/w d-state of Co, Ru, & Ni is greater in valance band than conduction band, this is because of s and p-states which contribute less in the TDOS PDOS of Co_2NiGe and Co_2RuGe compounds in the following figures. In the p-states of Ge of Co_2NiGe alloys contribute more into the valance band than the conduction band. In contrast, the p- orbital in Co_2RuGe contributes more to the conduction band than to the valance band

(Mouatassime et al., 2021). Since there is a discrepancy in the figures, the compounds behave somewhat metallically in nature.

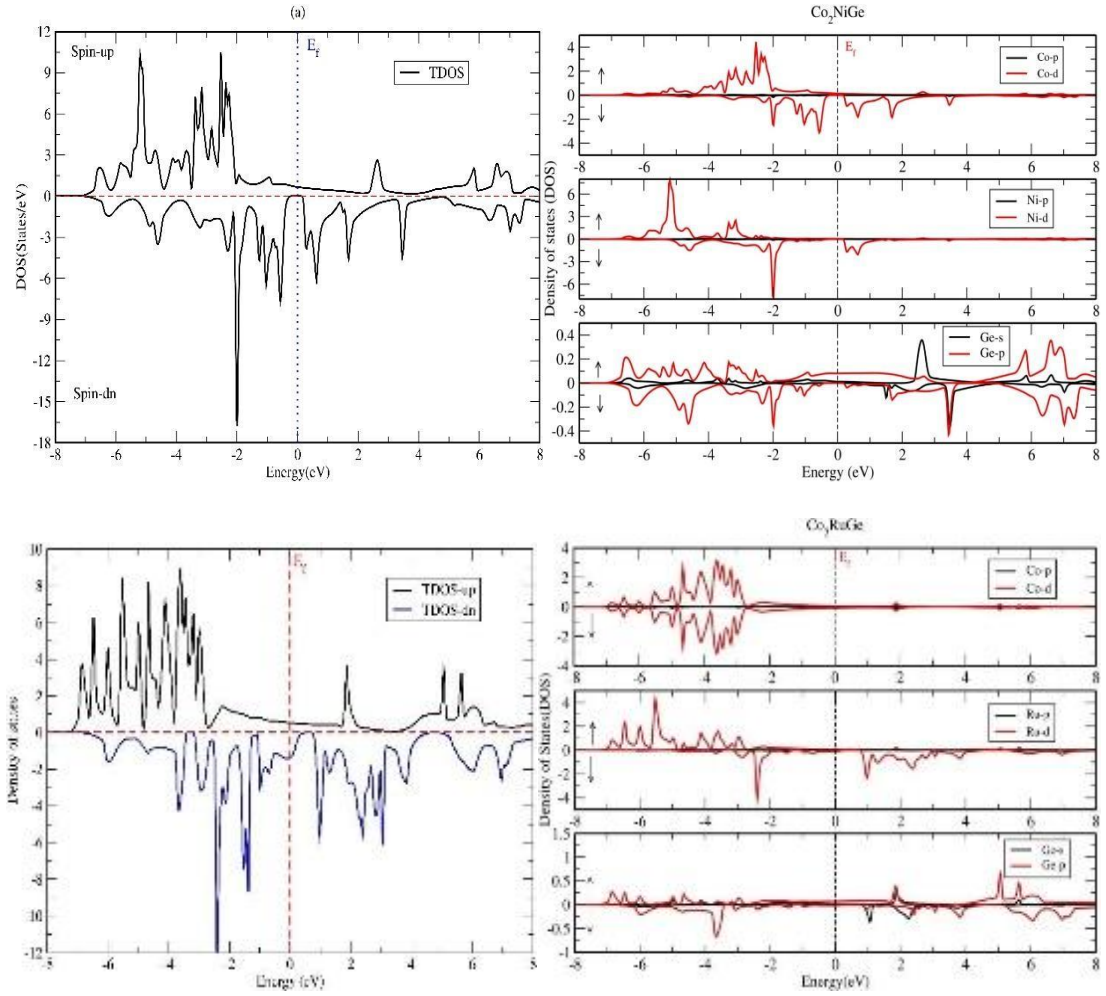

Figure 4: After applying PBE-GGA+U approximation on full Heusler alloys, get total DOS and PDOS of Co_2NiGe & Co_2RuGe.

3.3. Mechanical Properties

The elastic characteristics, including as stiffness, ductility, brittleness, and many more, are crucial in determining the mechanical stability of a compound (Colmenero, Fernández, Timón, & Cobos, 2018). The table below lists the computed values for the Full Heusler alloys Shear modulus Elastic parameters (Cij), Co2YGe(Y=Ni, Ru Bulk) modulus (B), (G), Young modulus (Y), Pugh ratio (B/G), Poisson ratio (V), and Debye temperature. Following are descriptions of how bulk and shear modulus cubic lattices of the Voigt Reuss-Hill calculated by elastic-parameters of a crystal: Young modulus: Y = 9BG/ (3B + G), Shear modulus: G = 1/2 (GV + GR), Young modulus: B = 1/3 (C11 + 2C12), and Poisson ratio: v = 3B2G/2(3B + G) (Ali & Rahaman, 2018). The table below displays the amounts above that have been calculated (C. Zhang et al., 2020). A thorough analysis of these quantities has been conducted in order to determine the harshness/ smoothness and linking characteristics of entire Heusler alloys Co_2YGe (Y=Ni, Ru). Packed Heusler alloys display a relatively high value of bulk-modulus while Half Heusler alloys display a low value of bulk modulus (Ilkhani et al., 2020). A compound can be more easily twisted if it has a high shear modulus value. The young modulus can then be determined from the computed values of the bulk and shear modulus. The power of the compound is represented by the elastic parameters. A high young modulus value indicates a higher mode of complexity. In this study, Co_2NiGe > Co_2RuGe is used to compare compounds with high stiffness. According to earlier research, a compound is considered elastically anisotropic if its Zener anisotropy value is more than 1 (A>1). On the other side, it is said to as elastically isotropic if its value is less than 1(A1).

Table 2
Studied elastic parameters of Co_2YGe Alloys where Y=Ni, Ru

Compounds	Co_2NiGe	Co_2RuGe
C11(GPa)	350.7453	134.0952
C12(GPa)	110.1819	125.2688
C44(GPa)	469.7302	65.2312
Bulk Modulus(B)	190.3697	128.21
Shear Modulus(G)	273.603	25.46
Young's Modulus(Y)	554.95	71.64
Pugh's Ratio	0.696	5.04
Poisson's Ratio	0.014	0.407
Debye Temp(K)	787.271	236.005

In above table, C11 denotes the composite alignment-related elasticity, and C12 and C44 denote the compound phase-change-related flexibility. We can determine mechanical of these compounds strength from their elastic properties. [36] Following are the cubic compounds for which the Born strength principle holds true: C11>0, C11+2C12>0, C11-C12>0, and C44>0. Elastic parameters of both compounds, for example Co_2NiGe & Co_2RuGe that were estimated in this work adhere by the mechanical strength-concept. After obtaining the necessary information on these elastic constants, we will be able to investigate the ductile and brittle characteristics of these compounds. The brittleness and ductility of the following compounds can be determined using methods such as C12-C44 (Cauchy pressure) (Dumre & Khare, 2022), B/G (Pugh ratio), and Poisson ratio. The ductility of the compound is shown here by Cauchy pressure. Cauchy pressure value must be greater than zero for a compound to be considered ductile.

On the other hand, the compound is referred to as fragile if its value is smaller than zero. The examined compounds in the subsequent work exhibit brittle natures due to their positive values (Wen et al., 2019). The second factor used to evaluate whether a chemical exhibits brittle or ductile behavior in nature is the Pugh ratio (B/G). Table 2 displays the results of the analysis of the bulk modulus to shear modulus for this determination. If the material in question has a Pugh ratio greater than 1.75, it is regarded as having ductile character. The third metric, the Poisson ratio (v), is utilized to determine if a compound is ductile or brittle. This parameter value must be larger than 0.26 for the compound to be considered ductile. It is said to be brittle in nature on the other hand, if its value is less than 0.26. This parameter in the subsequent work states that the compound Co_2NiGe is brittle by nature (Wen et al., 2019). While the ductile character of another combination, Co_2RuGe, is claimed. These details are all displayed in table 2.

3.4. Magnetic Properties

We estimated the total μB (magnetic moments) of the investigated compounds, like as Co_2NiGe alloys and Co_2RuGe alloys, as well as the μB of the Co, Ru, Ni, and Ge atoms in the Cu_2MnAl-type structure and the interstitial μB (magnetic moment) of the compounds, shown in table 3 (Wu, Kratzer, & Scheffler, 2007). We used the GGA approximation to obtain the values of the magnetic moment (Klaver, Olsson, & Finnis, 2007). Results show that because the compounds are half-metallic by nature, the predicted magnetic moments have higher values. The calculated findings are displayed in given table below.

Table 3
Calculated standards of Magnetic moments.

Alloys	Magnetic-moment Co	Magnetic-moment Y	Magnetic moment Ge	Magnetic Moment Interstitial	Magnetic moment(μB) Total
Co_2YGe (y=Ni)	1.62589	1.13681	0.05437	0.33452	3.99971
Co_2YGe (Y=Ru)	2.03241	2.59941	0.00408	0.11514	6.55317

4. Conclusions

DFT was utilized to examine the electrical, elastic, structural, and magnetic properties of complete Heusler alloys (Co_2YGe (Y=Ni, Ru)). The compounds structural

features reveal that Heusler alloys are excellent in L21 position by the face centered-cubic (FCC) structure and space group is Fm3m (no.225). The density of states and electronic band structure of these compounds demonstrate that they are semi-metallic (DOS). According to magnetic characteristics, the understudied substances are magnetic because they have a net magnetic moment. The properties of Co_2NiGe and Co_2RuGe are elastic, indicating their strength-filled nature. Co_2NiGe is brittle, whereas Co_2RuGe is ductile and highly rigid. These compounds exhibit half-metallic behavior and have higher stability, making them useful in a variety of applications like spintronic devices and quantum computing.

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