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On the subject

***Effect of uniaxial and hydrostatic stresses on Heusler alloys:
First-principles study.***

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Dedication

I dedicate this thesis to my beloved family, whose unwavering support, encouragement, and patience have been my foundation throughout this journey.

To my parents, for their endless sacrifices and belief in my potential.

To my siblings, for their love and inspiration.

And to all those who stood by me in times of doubt, this work is a tribute to your faith in me.

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Nomenclature

DFT	Density Functional Theory
SCF	Self-Consistent Field
GGA	Generalized Gradient Approximation
PBE	Perdew–Burke–Ernzerhof Exchange-Correlation Functional
mBJ	Modified Becke–Johnson Potential
FP-LAPW	Full-Potential Linearized Augmented Plane Wave Method
DFPT	Density Functional Perturbation Theory
DOS	Density of States
TDOS	Total Density of States
PDOS	Partial Density of States
EF	Fermi Energy (Fermi Level)
SOC	Spin-Orbit Coupling
NM	Non-Magnetic
FM	Ferromagnetic
GMR	Giant Magnetoresistance
TMR	Tunnel Magnetoresistance
MTJ	Magnetic Tunnel Junction
MRAM	Magnetic Random Access Memory
TC	Curie Temperature
RMT	Muffin-Tin Radius
EOS	Equation of State

General Introduction

Spintronics, often referred as spin electronics, represents a subfield of nanoscience that emerged following the discovery of giant magnetoresistance (GMR) in 1988. This method, in contrast to typical electronics, leverages the quantum characteristic of electron spin to store information.

Classical electronics relies on a basic characteristic of electrons: electric charge. However, this domain faces challenges related to miniaturization, due to a physical limit that cannot be surpassed without reassessing the foundational principles of electronics. Utilizing the second characteristic of electrons, known as spin, we could potentially exceed this boundary while maintaining the fundamental methods of classical electronics. A major advancement in this field was the discovery of giant magnetoresistance, which awarded Albert Fert [\[1\]](#) and Peter Grünberg [\[2\]](#) the Nobel Prize in Physics in 2007.

Currently, this phenomenon is applied in spin valves [\[3\]](#). These devices consist of two ferromagnetic layers (electrodes) that are divided by a thin metal spacer (barrier), leading to electrical resistance that varies based on the magnetic arrangement of the electrodes. By introducing a weak magnetic field, we can adjust the magnetizations of the electrodes, leading to two distinct configurations: the parallel configuration, in which the magnetizations are aligned in the same direction, producing low electrical resistance, and the antiparallel configuration, where the magnetizations are oriented in opposing directions, causing an increase in electrical resistance. One of the most well-known applications of this technology is the giant magnetoresistance (GMR) effect reading head [\[4\]](#) utilized in modern hard drives.

The evolution of spin valves into magnetic tunnel junctions (MTJs) has occurred by replacing the metallic barrier with an insulating barrier. This advancement has led to the discovery of tunnel magnetoresistance (TMR) [\[5\]](#), which was first discovered by Mr. Jullière in 1975.

As our understanding of the mechanisms involved in MTJs [6] has advanced, we have successfully identified the elements that influence the performance of these devices. MTJs now form the foundation for cutting-edge spintronic components, particularly in the advancement of future random-access magnetic memory (MRAM) hard drives.

In these devices, the probability of an electron traversing the insulating barrier is contingent upon its spin and the orientation of the magnetization in the magnetic layers. Similar to spin valves, when arranged in a parallel configuration, the electrical resistance is reduced in comparison to an antiparallel configuration. This phenomenon occurs because electrons can only cross the barrier via tunneling, a process influenced by their spins and the symmetry of their wave functions.

Data storage can be achieved via spin, which refers to a magnetic bit (0 or 1) defined by the parallel or antiparallel orientations of a magnetoresistance device (such as spin valves or magnetic tunnel junctions). To access information, the electrical resistance of the device can be assessed (measured) to determine its state. Writing to memory is feasible by applying a weak magnetic field to align one of the magnetic layers.

Nevertheless, this type of architecture may restrict information density. A potential solution to this challenge is to inject a spin-polarized current directly into the device, a method referred to as spin transfer. The integration of spin transfer with MRAM has resulted in the creation of STT-MRAM (Spin Transfer Torque MRAM), marking a notable progress in this domain.

The essential elements of spin valves and magnetic tunnel junctions consist of thin layers of ferromagnetic materials.

In the framework of developing these devices for spintronic applications, magnetic semiconductors represent a promising class due to their potential to combine semiconducting behavior with intrinsic magnetic ordering. In this thesis, we investigated several magnetic

semiconductor compounds to understand and compare their structural stability, electronic band structures, and magnetic properties. Our goal is to identify materials that not only exhibit robust ferromagnetism but also maintain favorable electronic characteristics compatible with device integration thus contributing to the rational design of next-generation spintronic materials.

Although numerous Heusler compounds have been theoretically predicted and experimentally synthesized, the influence of external parameters such as hydrostatic and uniaxial pressure on their physical properties remains an active area of research. Pressure engineering represents an effective approach for tuning the interatomic distances and modifying the electronic structure, magnetic interactions, and phase stability of materials without changing their chemical composition.

The primary objective of this thesis is to investigate the effects of hydrostatic and uniaxial pressure on selected Heusler magnetic semiconductors using first-principles calculations based on Density Functional Theory (DFT). Particular attention is devoted to understanding the evolution of the structural stability, electronic band structure, magnetic behavior, and dynamical stability under different pressure conditions.

The present work focuses on two representative systems: the quaternary Heusler compound CoMnTaSb and the full-Heusler family Rb_2TiZ ($Z = \text{Si, Ge, Sn, and Sb}$). For these compounds, we aim to determine their equilibrium structural properties, evaluate their thermodynamic, mechanical, and dynamical stability, and analyze their electronic and magnetic characteristics. Furthermore, the influence of hydrostatic and uniaxial pressure on the band-gap evolution, magnetic moments, and spin-dependent electronic properties is systematically examined.

Through this study, we seek to clarify the mechanisms governing pressure-induced modifications in Heusler magnetic semiconductors and to assess their potential for future

spintronic and magnetoelectronic applications. The obtained results may also provide useful guidelines for the design and optimization of novel pressure-tunable functional materials.

In addition, the Rb_2TiZ ($Z = \text{Si, Ge, Sn, and Sb}$) full-Heusler compounds were investigated as promising magnetic semiconductors, with particular emphasis on the response of their electronic and magnetic properties to hydrostatic and uniaxial pressure."This thesis is divided into three chapters organized in the following manner:

The first chapter introduces a distinct class of Heusler compounds, outlining their crystalline structures, fundamental characteristics, and potential technological applications.

The second chapter explores the influence of strain on Heusler materials, examining how hydrostatic, uniaxial, and biaxial strains affect their structural, electronic, magnetic, and optical properties. It also discusses the underlying physical mechanisms and highlights key findings from recent theoretical and experimental studies.

The final chapter presents and analyzes the obtained computational results, providing an overview of the methods employed and their application to the studied compounds. In conclusion, a comprehensive summary emphasizes the main findings and proposes future research directions, particularly regarding the integration of these materials into spintronic devices.

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Chapter I

Heusler Alloys

I.1 Introduction:

The quest for innovative materials in spintronics has led to the emergence of a new category of compounds referred as Heusler compounds. For approximately three decades, these materials have been favored for various applications due to their tunable electronic structures. Furthermore, they possess a broad spectrum of physical properties. This versatility allows for the design of materials with specific desired traits, including half-ferromagnetic metals. [1, 2] to antiferromagnets [3], non-magnetic semiconductors [4, 5], and even superconductors [6, 7]. Among which, we can name a few: ferromagnetic (Cu_2MnAl [8]), ferrimagnetic (Mn_2VAl [9]), semiconductors (Fe_2VAl [10]), heavy fermion systems (Cu_2CeIn [11]), and the superconductors (Ni_2ZrGa [12]).

Over 3,000 Heusler compounds have been identified, showcasing potential applications across various fields such as spintronics, optoelectronics, and magneto-optics. Recently, new applications have surfaced, including environmental technologies like thermoelectric devices [13, 14] and the solar cell technology [15], the recent discovery of topological insulators has also unveiled a new state of quantum matter. These intriguing properties pave the way for future technologies with countless possibilities for utilizing Heusler compounds [16, 17].

This chapter provides an overview of Heusler alloys since their discovery, detailing the various possible structures, key properties as well as areas of application.

I.2 Heusler alloys history:

Heusler compounds are exemplified by the alloy Cu_2MnAl , which was initially identified by Friedrich Heusler in 1903 [8]. The crystal structure of this alloy was later examined by Bradley and Rodgers in 1934 [18]. Cu_2MnAl demonstrated ferromagnetic properties and possesses a high Curie temperature. Indeed, their characteristics are entirely distinct from their composed elements.

For instance, the alloy Cu_2MnAl is a magnetic compound despite the fact that copper (Cu), manganese (Mn), and aluminium (Al) do not exhibit magnetism independently [8,19]. Likewise, the alloy TiNiSn [13, 20] performs as a semiconductor, even though it is built of three metallic elements [21]. In other words, Heusler alloys are ternary ferromagnetic compounds. Research conducted in 1963 revealed that manganese is crucial to the total magnetic moment of the alloy Cu_2MnSb [22].

It is notable that pure manganese (Mn) displays antiferromagnetic type. The magnetic characteristics of Heusler compounds are significantly affected by their crystal structure, as the atomic arrangement between them gives rise to ferromagnetism.

This prior research has led to the emergence of an intriguing (captivating) new category of materials, known as Heusler compounds, which encompasses more than 3,000 distinct compounds. These compounds are denoted by the general chemical formula X_2YZ , where X and Y represent transition metals and Z is either a semiconductor or a non-magnetic metal. The extensive variety of compounds that can be created by combining nearly all elements from the periodic table is outlined in *Figure I.1*.

X₂YZ

Heusler compounds

H 2.20																	He	
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne	
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar	
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00	
Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.60	Mo 2.16	Tc 1.90	Ru 2.20	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.10	I 2.66	Xe 2.60	
Cs 0.79	Ba 0.89			Hf 1.30	Ta 1.50	W 1.70	Re 1.90	Os 2.20	Ir 2.20	Pt 2.20	Au 2.40	Hg 1.90	Tl 1.80	Pb 1.80	Bi 1.90	Po 2.00	At 2.20	Rn
Fr 0.70	Ra 0.90																	
		La 1.10	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.20	Gd 1.20	Tb 1.10	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.10	Lu 1.27		
		Ac 1.10	Th 1.30	Pa 1.50	U 1.70	Np 1.30	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.30	Cf 1.30	Es 1.30	Fm 1.30	Md 1.30	No 1.30	Lr 1.30		

Figure I.1: Periodic table of the elements. The vast number of Heusler materials can be formed by combining different elements according to a specific color scheme.

I.3 Nomenclature of Heusler Compounds:

I.3.1 Half Heusler Compounds:

These alloys possess a chemical composition within the general formula XYZ. In 1983, Groot and his team [23] identified a half-Heusler alloy of the NiMnSb [24] variety. Half-Heusler alloys can be described as compounds made up of two components with differing properties: one being covalent and the other ionic. Consequently, the atoms X and Y display different cationic characteristics, while Z serves as the anionic counterpart [25].

The nomenclature found in the literature does not adhere to an alphabetical sequence for the elements, nor is it arbitrary; rather, it is determined by their electronegativity. The most electropositive element is positioned at the start of the formula. This element may be a main group element, a transition metal, or a rare earth element. In contrast, the most electronegative element is located at the end of the formula and is usually a main group element from the latter half of the periodic table. Examples of such compounds include LiAlSi, ZrNiSn, and LuAuSn [26,27].

I.3.2 Full Heusler compounds:

Heusler alloys, commonly known as full-Heusler alloys, belong to a category of intermetallic compounds. These alloys are characterized by the general formula X_2YZ , where X and Y represent transition metals, and Z is an element from groups III, IV, or V of the Mendeleev periodic table. There are notable exceptions where this formula may differ.

For example, the element Y can occasionally be a rare earth element or an alkaline earth metal. A typical example of a full-Heusler alloy is Co_2MnSi , and another is Fe_2VAl [28,29]. In these instances, the metal (X) is represented in two parts, positioned at the start of the formula as the most electropositive component, while the most electronegative element is found at the end.

Nevertheless, there are exceptions where certain elements are deemed more electropositive. For instance, in the compounds LiCu_2Sb and YPd_2Sb [30], the electropositive element is placed at the beginning of the formula in accordance with IUPAC nomenclature (International Union of Pure and Applied Chemistry).

I.4 Heusler alloys crystal structure:

Heusler alloys are divided into two primary families according to their crystal and atomic structures. This categorization emphasizes the arrangement of atoms within the crystal lattice, which has a substantial impact on their properties. Even slight disorder in atomic distribution can greatly modify electronic structure, magnetic properties, and transport properties [31,32].

Half-Heusler alloys possess ordered atomic configurations referred to as C1_b and L2_1 structures, whereas full-Heuslers exhibit a Y-type structure. Disordered atomic configurations encompass types A2, B2, DO3, and B32a.

I.4.1 Half Heusler crystal structure:

The alloys belonging to this family are characterized by a chemical composition referred to as XYZ. Half-Heusler alloys are ternary intermetallic compounds consisting of two transition metals, X and Y, along with Z, which serves as a valence s-p element. These alloys crystallize in a cubic C1_b structure; however, one of the four unoccupied sublattices may remain vacant, permitting a vacuum to substitute for one of the X atom lattices located at the c2 positions of the L2_1 structure.

Experimental findings validated this feature via infrared absorption [33] and spin-resolved positron extermination [34,35].

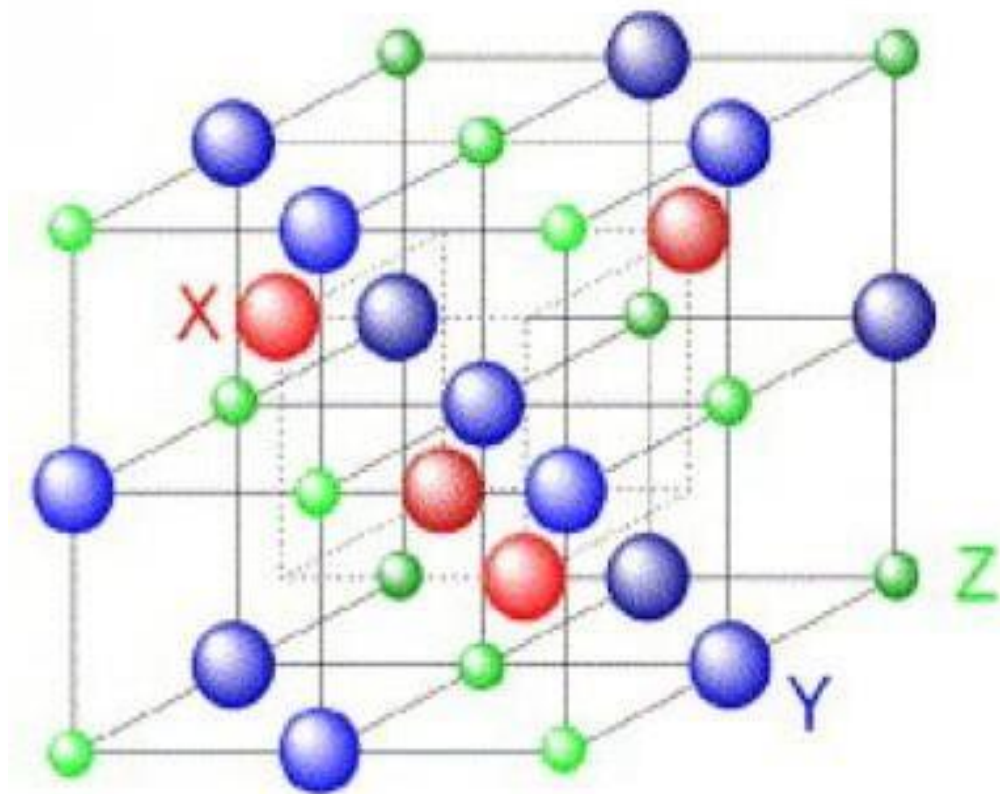


Figure I.2: Half-Heusler crystal structure

Table I.1 details the various forms of atomic disorder found in the half-Heusler structure $C1_b$ [36], incorporating notations from the Inorganic Crystal Structure Database (ICSD). It provides structural documentation from "Proud Skins" (SB), the Pearson database, along with the relevant space groups for these Heusler alloys.

Table I.1. Site occupancy, general formula, structural type (based on various databases) for different atomic arrangements and the space group of half-Heusler compounds.

Site occupation	General formula	Structure type			Space group
		ICSD	SB	Pearson	
4a,4b,4c	XYZ	LiAlSi	C1 _b	cF16	F-43m 216
4a= 4b,4c	XY ₂	CaF ₂	C1	cF12	Fm-3m 225
4a,4b, 4c=4d	X ₂ YZ	Cu ₂ MnAl	L2 ₁	cF16	Fm-3m 225
4a=4b, 4c=4d	XZ	CsCl	B2	cP2	Pm-3m 225
4a=4c, 4b=4d	YZ	NaTl	B32a	cF16	Fd-3m 227
4a= 4b= 4c=4d	X	W	A2	cI2	Im-3m 229

I.4.2 Full Heusler Crystal structure:

Full-Heusler alloys are mainly recognized for their L2₁ structure, which features a systematic arrangement of atoms. Nevertheless, there are also other disordered structures like Y, A2, DO3, and B2 [43=37]. This disorder can greatly influence the electronic, magnetic, and transport properties of alloys [31.32].

Numerous structures are recorded in the Inorganic Crystal Structure Database (ICSD), Cambridge Structural Database (CSD), and Pearson's database [37,38,39], as outlined in **Table**

I.2.

Table I. 2. Full Heusler compounds different structures.

Site occupation	General formula	Structure type			Space group
		ICSD	SB	Pearson	
X, X', Y, Z	XX'YZ	LiMgPdSn	Y	cF16	F-43m 216
X=X', Y, Z	X ₂ YZ	Cu ₂ MnAl	L2 ₁	cF16	Fm-3m 225
X, X'=Y, Z	XX' ₂ Z	CuHg ₂ Ti	X	cF16	F-43m 216
X=X'=Y, Z	X ₃ Z	BiF ₃	DO ₃	cF16	Fm-3m 225
X=X', Y=Z	X ₂ Y ₂	CsCl	B2	cP2	Pm-3m 221
X=Y, X'=Z	X ₂ X' ₂	NaTl	B32a	cF16	Fd-3m 227
X=X'=Y=Z	X ₄	W	A2	Cl2	Im-3m 229

The crystal structures linked to different types are illustrated in **Figure I.3** [40], which are elaborated upon in the subsequent paragraphs.

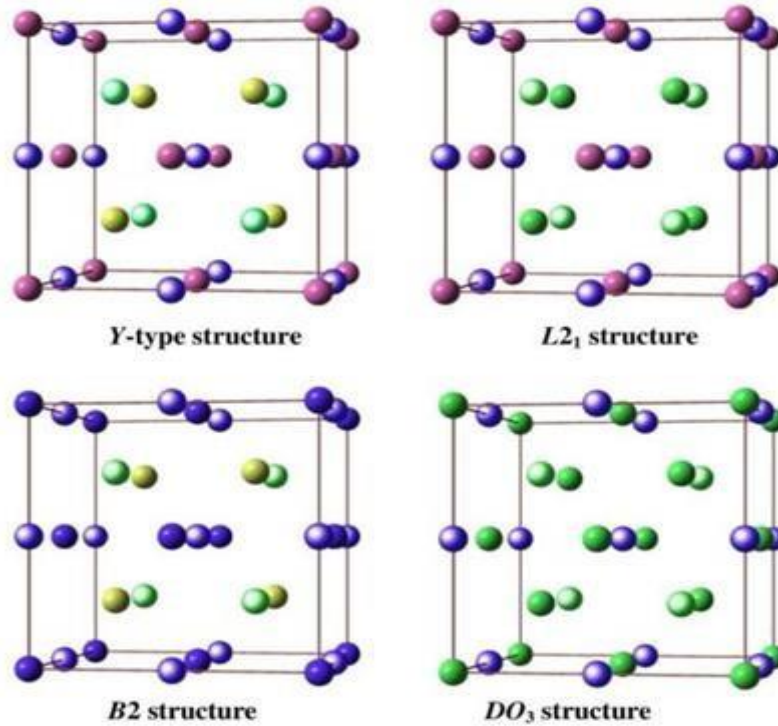


Figure I.3 Full Heusler crystal structure.

The blue, purple, yellow, and green circles denote the positions 4a (0, 0, 0), 4b (1/2, 1/2, 1/2), 4c (1/4, 1/4, 1/4), and 4d (3/4, 3/4, 3/4), respectively. In the case of quaternary Heusler compounds, there are two distinct elements, X and X', which occupy the 4a and 4d positions, respectively. The element Y is situated at position 4b, while Z is found at position 4c. This structure is modelled after the prototype LiMgPdSn [41]. An illustration depicting the inverse Heusler structure [42] alongside the quaternary variant can be found in **Figure I.4**

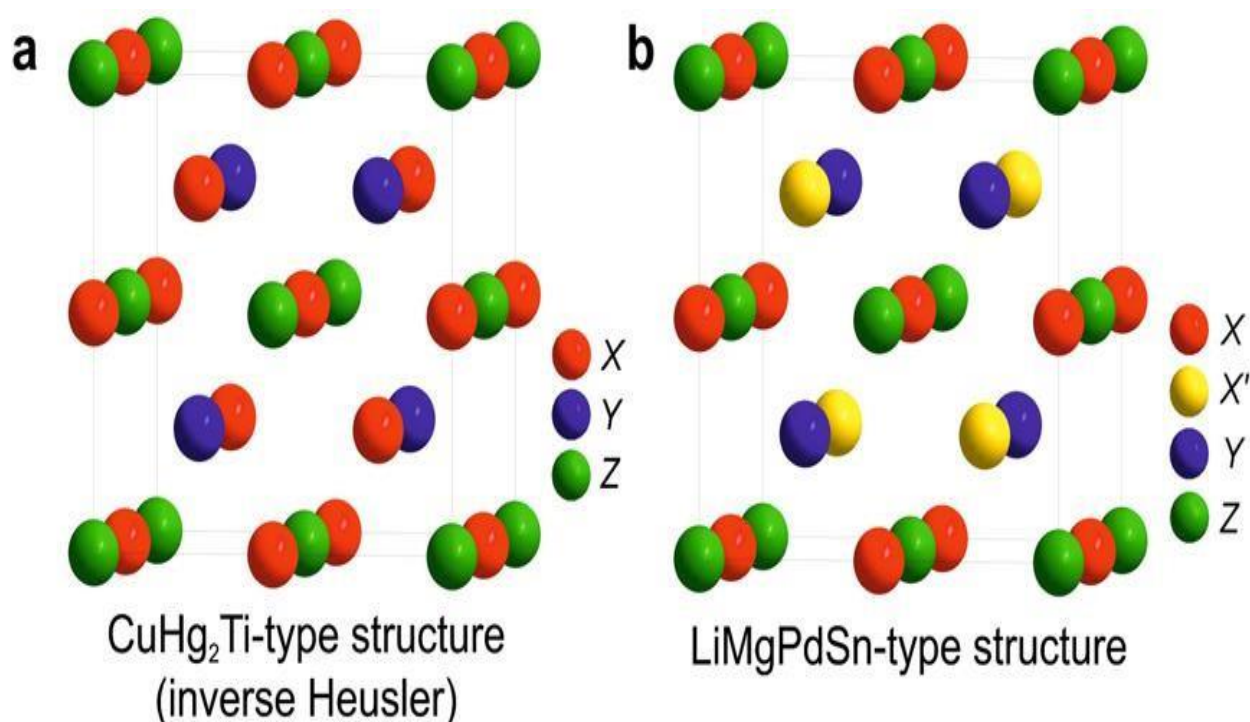


Figure I.4: (a) The inverse Heusler structure CuHg_2Ti and (b) the quaternary version LiMgPdSn .

I.5 Slater-Pauling rule:

In transition metals and their alloys, the atomic energy levels of 3d and 4s expand to form a band structure, where the density of states in the d band surpasses that of the s band close to the

Fermi level (EF). The interaction of d-orbitals from adjacent atoms results in a rivalry between electronic correlations that tends to locate electrons and their kinetic energy band.

Cobalt-based Heusler alloys are intermetallic compounds composed of 3d transition metals that display localized magnetism. Their magnetic moments adhere to a specific pattern determined by the number of valence electrons and the crystal structure, a phenomenon referred as Slater-Pauling behavior [43,44,45].

In half-Heusler half-metallic alloys featuring a C1_b structure, the total magnetic moment can be represented by the equation: $M_t = Z_t - 18$, where Z_t denotes the number of valence electrons, derived from the sum of spin-up and spin-down electrons.

$$Z_T = \uparrow + \downarrow, \mu_{\uparrow} = \uparrow - \downarrow, \mu_{\downarrow} = \downarrow - 2\uparrow$$

Due to the full occupation of the nine minority bands, we suggest a rule for estimating the total magnetic moment of half-Heusler alloys, which consist of three atoms per formula unit and exhibit half-metallic properties.

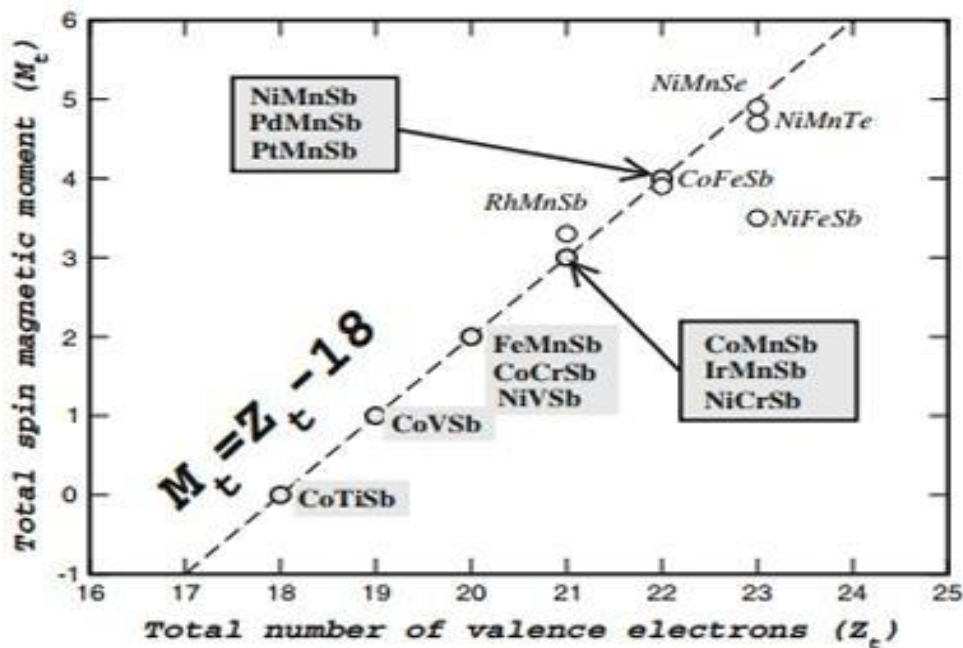


Figure 1.5 Half Heusler Slater Pauling curves.

Figure I.5 illustrates the computed total magnetic moments as a function of the total number of valence electrons. Compounds situated along the dotted diagonal adhere to the rule:

$$M_T = Z_T - 18$$

where M_T represents the total magnetic moment (integer value) and Z_T denotes the total number of valence electrons.

When Z_T is 18 or more, the total magnetic moment varies from 0 to 5 μ_B . A value of 0 signifies a semiconductor phase, whereas a value of 5 indicates that all 10 majority d states are filled; however, the nearly half-metallic behavior is determined.

Subsequently, we will demonstrate the behavior of Slater-Pauling for the full-Heusler alloys.

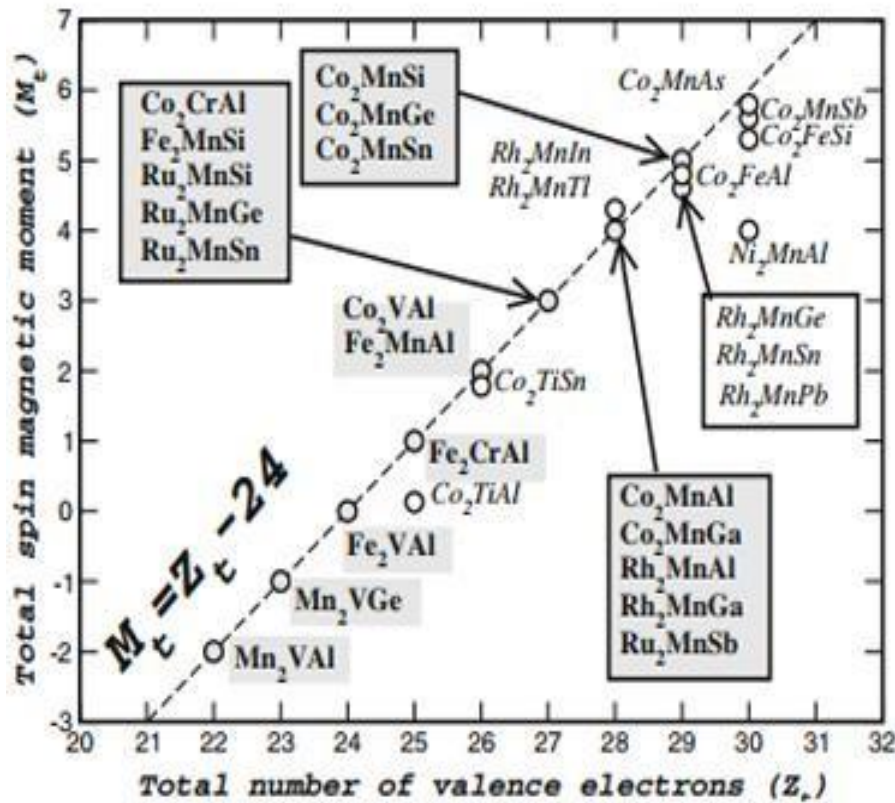


Figure I.6 Full Heusler Slater Pauling curves.

Figure I.6 illustrates the total magnetic spin moments as a function of the total number of valence electrons for all full-Heusler compounds.

The dashed line signifies the half-metallicity rule:

$$\mathbf{M_T = Z_T - 24}$$

which suggests that the minority band comprises 12 electrons per unit cell: 4 in the lower energy levels of the s and p orbitals, and 8 in the minority bands of the Co atom (2 e_g , 3 t_{2g} , and 3 t_{1u}).

As a result, the 7 unoccupied minority bands permit a maximum magnetic moment of 7 μ_B when all majority states are occupied (see **Figure I.7**).

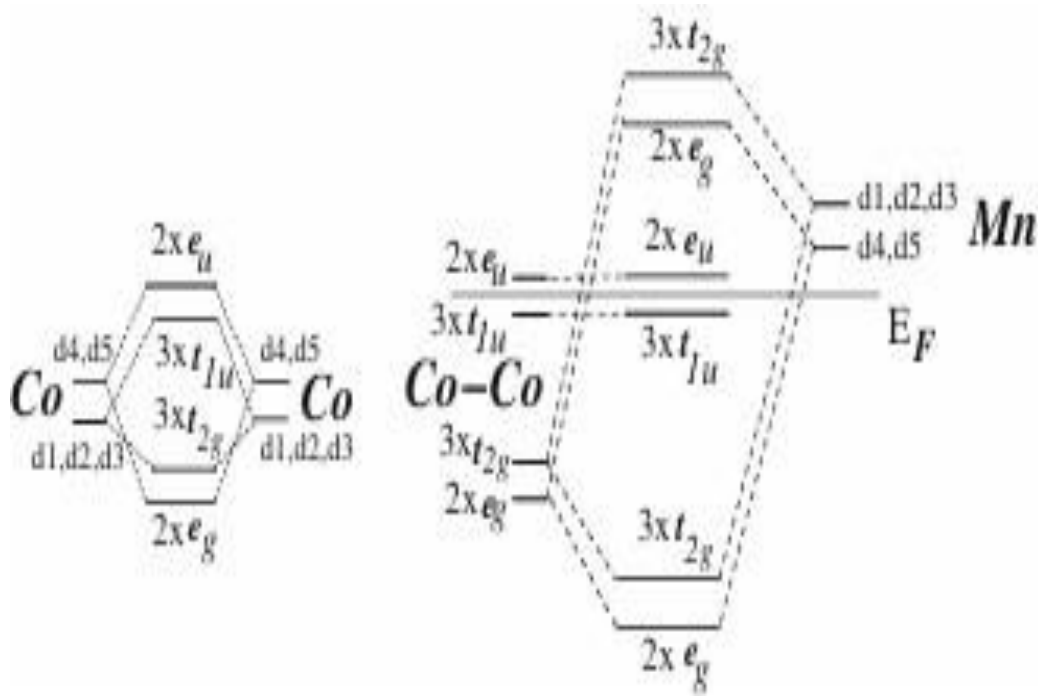


Figure I.7 Schematic illustration of the origin of the gap in the minority band in full-Heusler alloys.

Consequently, utilizing the number of valence electrons per formula unit is a more practical approach for calculating the total magnetic moment of half-metallic Heusler compounds:

Half-Heusler compounds (XYZ) consist of three atoms per formula unit, and their total magnetic moment adheres to the Slater-Pauling rule at 18, known as the "rule of 18". In contrast, full-Heusler compounds (X_2YZ) contain four atoms per unit, and their total magnetic moment conforms to the Slater-Pauling rule at 24, referred to as the "rule of 24".

I.6 Magnetic semiconductors:

Magnetic semiconductors are materials that demonstrate both semiconducting characteristics and magnetic properties. These materials can offer novel functionalities for spintronic and magnetoelectronic devices; for instance, they can act as spin-filter materials.

Among the Heusler compounds, two families have recently been investigated as magnetic semiconductors suitable for use as spin-filter materials: (CoV)XAl, where X can be Ti, Zr, or Hf, which are categorized as ferromagnetic semiconductors, and (CrV)XAl, with X also being Ti, Zr, or Hf, which are classified as fully compensated ferrimagnetic semiconductors.

In **Figure I.8** we present the total density of states for (CoV)TiAl and (CrV)TiAl where the energy gaps in both spin-directions are present.

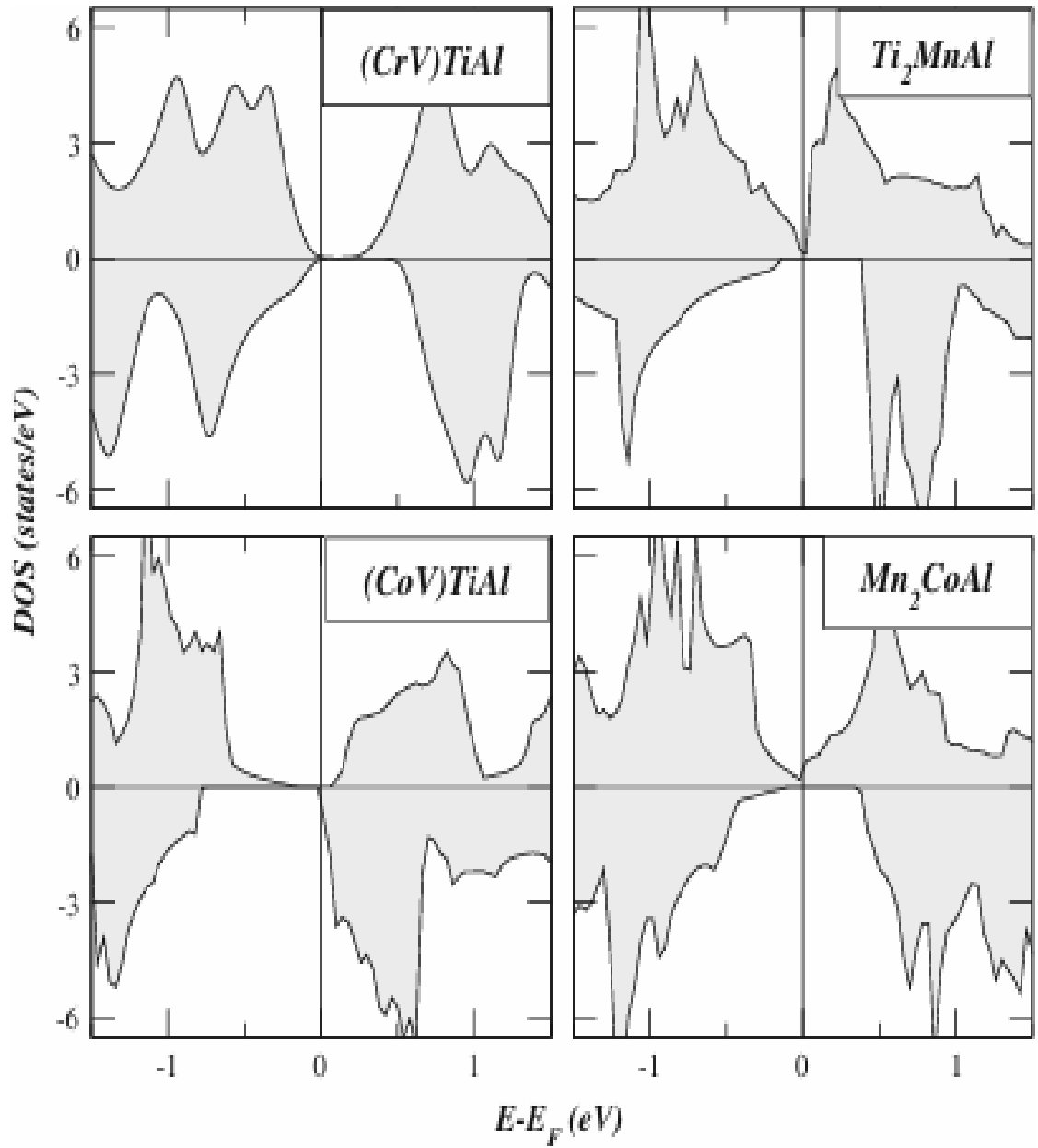


Figure I.8 Total DOS per formula unit around the Fermi level for four magnetic semiconductors. $(\text{CrV})\text{TiAl}$ is a fully-compensated ferrimagnetic semiconductor, $(\text{CoV})\text{TiAl}$ is a ferromagnetic semiconductor, and Ti_2MnAl and Mn_2CoAl show a spin-gapless semiconducting behavior.

I.7 Conclusion:

In this chapter, we present the context of this thesis, with a particular emphasis on Heusler alloys. We define these alloys and review various studies regarding their properties, highlighting their extensive and dynamic characteristics.

The investigation of these alloys represents a recent advancement when compared to the abundance of theoretical predictions and experimental studies that exist. Our focus is on the theoretical analysis of magnetic semiconductors, which have the potential to function as ferromagnetic half-metals. These alloys conform to the Slater-Pauling rule. Such attributes emphasize their promise in the cutting-edge domains of spintronics and optoelectronics.

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Chapter II

Stresses Effect on Materials

II.1 Introduction:

Internal stresses arise when external loads are applied to a material sample, resulting in deformation and alterations in shape and volume. These stresses, which may persist even after the load is removed, are referred to as residual stresses. They have a significant effect on mechanical properties, affecting processes such as fracture, crack propagation, fatigue, and recrystallization. In certain cases, residual stresses can improve material characteristics, for instance, by enhancing resistance to cracking through the application of compressive stress.

Residual stresses can be assessed using a variety of techniques, including destructive methods like layer removal and non-destructive approaches such as ultrasonic techniques and Raman spectroscopy. The diffraction method is especially beneficial due to its non-destructive nature and its capability to analyze both macro and micro stresses in multiphase materials. While traditional X-ray methods can only investigate residual stresses to a depth of a few micrometers, synchrotron or neutron radiation enables analysis at depths of several centimeters and throughout the entire volume of the sample. This study utilizes both classical X-ray and neutron diffraction techniques to investigate stress fields in polycrystalline materials, addressing the impact of different types of stress on diffraction outcomes.

Experimental methods like diffraction provide valuable insights into the stress distribution in materials. In contrast, Density Functional Theory (DFT) offers a detailed, atomistic, and electronic-level perspective that deepens our understanding of the origins and effects of stress. By combining diffraction techniques with DFT simulations, we can achieve a more comprehensive analysis: experimental data can validate theoretical predictions, while theoretical models can explain phenomena that are challenging to investigate experimentally.

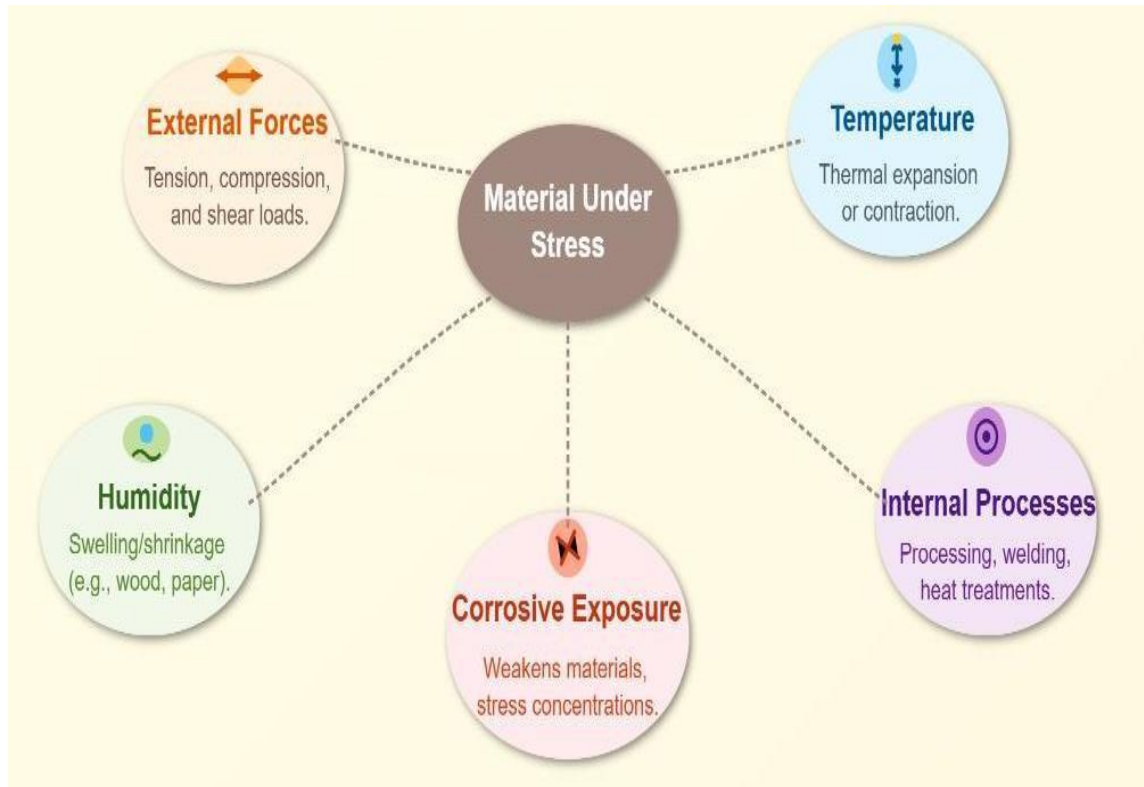


Fig.II.1. Internal stresses in materials.

II.2 Strain Influence on Heusler Materials

The strain effect in Heusler materials provides a powerful way to control and enhance mechanical stability, electronic structure, thermoelectric performance, and magnetic properties, making these materials versatile for applications in thermoelectric and spintronics.

This understanding comes from density functional theory studies, experimental thin-film investigations, and advanced spectroscopic techniques revealing strain-induced orbital and lattice modulations specific to Heusler systems.

Applying tensile or compressive strain can alter the lattice constants and induce tetragonal distortion in Heusler alloys. For example, isotropic strain in half-Heusler compounds like BiBaK affects their elastic and phonon properties while maintaining mechanical and thermodynamic stability under different strain levels. In thin films of Co-based Heusler

alloys, strain changes from tensile to compressive when buffer layers are introduced, affecting the tetragonal distortion magnitude.

Strain modifies the electronic band structure and bandgap of Heusler materials. Compressive strain often increases the bandgap, while tensile strain decreases it, impacting materials' semiconducting or metallic behavior. These changes in electronic structure affect thermoelectric performance, as seen in BiBaK, where compressive strain enhances the thermoelectric figure of merit.

II.3 Current State of Knowledge

In general, hydrostatic pressure induces a phase transition in Heusler alloys, extending the operational temperature range toward higher values and shifting the optical absorption spectra to higher energies (within the visible region). This phenomenon tends to preserve or even enhance the intensity of optical responses such as absorption.

In DFT calculations, hydrostatic pressure is modeled by an isotropic reduction of the crystal cell volume followed by atomic relaxation. The equations of state (Murnaghan, Birch-Murnaghan) describe the relationship between pressure (P), volume (V), and the bulk modulus.

$$P(V) = \frac{3}{2}B_0 \left[\left(\frac{V_0}{V} \right)^{7/3} - \left(\frac{V_0}{V} \right)^{5/3} \right] \left\{ 1 + \frac{3}{4}(B'_0 - 4) \left[\left(\frac{V_0}{V} \right)^{2/3} - 1 \right] \right\}$$

In reference [1], the electronic structure analysis of Fe₂TaAl and Fe₂TaGa reveals that both materials exhibit semiconducting behavior, with band gaps of approximately 0.84 eV and 0.64 eV, respectively. Under applied pressure, a transition from an indirect to a direct band gap is observed at around 5 GPa and 80 GPa, respectively. Phonon dispersion calculations

further confirm that both materials remain dynamically stable within the investigated pressure range. Regarding their optical properties, increasing pressure results a blue shift of the optical conductivity spectra. On the other hand, the application of anisotropic strain exhibit distinct effects. For instance, in FeVSb half-Heusler alloy [2], uniaxial stress induces a structural phase transition at relatively low pressure (around 0.5 GPa) from a cubic to a hexagonal structure. This transition is accompanied by a reduction in optical performance, including the decrease in the intensity of optical absorption peaks, as well as reductions in both the static dielectric constant and refractive index along the stressed direction. Unlike hydrostatic pressure, uniaxial stress does not lead to a significant shift in absorption peaks but primarily reduces their intensity, revealing the stronger anisotropic influence on the electronic and optical properties of the material. In another study [3] the quaternary Heusler compound LiScNiGe was investigated using density functional theory (DFT) under pressure ranging from 0 to 100 GPa. The results indicate that the compound remains mechanically and dynamically stable, while its band gap significantly increases from 0.647 eV to 1.437 eV, suggesting pressure-induced enhancement of semiconducting behavior. Similarly, the quaternary ScNiCrX (X = Al, Ga) Heusler alloys [4] have been studied under pressure up to 10 GP, where the calculated total magnetic moment, M_T (for both alloys) follows the Slater-Pauling rule, $M_T = (N_V - 18) \mu_B$. Up to 6.0 GPa, it is expected that the ScNiCrAl alloy to show 100% spin-polarization (at the Fermi-level, E_F), whereas for the ScNiCrGa, complete spin-polarization can be maintained up to 16.0 GPa.

Furthermore, the Rh₂MnAl full-Heusler alloy [5] has been examined under both hydrostatic and uniaxial strains, demonstrating adherence to the Slater–Pauling rule with a total magnetic moment 4.000 μ_B at strain of 5.7 and 10.2%, respectively. In reference [6] Authors reported that CaFe₂As₂ exhibits a unique phase transition from a magnetic orthorhombic phase to a nonmagnetic collapsed tetragonal phase under both hydrostatic and uniaxial pressures, with no

evidence of an intermediate tetragonal phase under uniaxial conditions. In contrast, BaFe₂As₂ undergoes two successive phase transitions from a magnetic orthorhombic to a collapsed tetragonal phase via an intermediate nonmagnetic tetragonal state under both types of applied pressure. Finally, for the X₂RuPb (X = Sc, Y, La) series, a topological phase transition has been identified, evolving from a trivial semiconducting to a nontrivial topological insulating state. This transition arises from the electronic band inversion mechanism, strongly influenced by spin–orbit coupling and modulated by both hydrostatic and uniaxial strains.

II.3.1 Bulk Modulus, Compressibility and Equation of State

The response of a material to external pressure is commonly characterized by two fundamental quantities: the bulk modulus and the compressibility. These parameters provide valuable information about the resistance of a crystal structure to volume changes under compression and are widely used to evaluate the mechanical stability of materials.

The isothermal bulk modulus is defined as:

$$K_T = -V \left(\frac{\partial P}{\partial V} \right)_T$$

where V is the volume and P is the applied pressure. A larger bulk modulus indicates a stronger resistance to compression and therefore a higher structural rigidity.

The inverse quantity, known as the compressibility, is expressed as:

$$\beta = 1/K$$

and describes the relative change in volume produced by a variation of pressure. Materials with low compressibility generally exhibit high bulk modulus values and enhanced resistance to external stresses.

In pressure-dependent studies, these parameters play an important role in understanding the structural behavior of materials. For Heusler compounds, the bulk modulus provides useful

information regarding their mechanical rigidity and structural stability, while the compressibility reflects their sensitivity to external compression. Variations in these quantities may significantly influence interatomic distances, electronic interactions, and magnetic coupling mechanisms.

II.3.2 Physical Effects of Hydrostatic and Uniaxial Pressure on Electronic and Magnetic Properties

External pressure constitutes an effective approach for tuning the physical properties of materials without altering their chemical composition. By modifying the interatomic distances within the crystal lattice, pressure affects the overlap between atomic orbitals and consequently influences the electronic and magnetic behavior of the system.

Under hydrostatic pressure, the crystal undergoes a uniform compression in all crystallographic directions. This isotropic reduction of the lattice volume generally enhances orbital hybridization and modifies the electronic band structure. As a consequence, important characteristics such as the band gap, density of states, and charge distribution may experience significant changes. Depending on the nature of the material, hydrostatic pressure can either increase or decrease the band gap and may even induce electronic phase transitions.

In contrast, uniaxial pressure generates an anisotropic deformation because the compression is applied along a specific crystallographic direction. This directional distortion alters the electronic structure differently along the various crystallographic axes, leading to modifications in band dispersion and electronic anisotropy. Therefore, uniaxial pressure offers an additional degree of freedom for controlling the electronic properties of materials.

The magnetic properties are also strongly influenced by pressure since magnetic exchange interactions depend sensitively on interatomic spacing. Changes in atomic distances modify the overlap between magnetic orbitals, which may affect both the magnitude of atomic magnetic moments and the strength of magnetic coupling. Consequently, pressure engineering

has become a powerful strategy for tailoring the electronic and magnetic properties of Heusler compounds intended for spintronic applications.

For this reason, investigating the influence of hydrostatic and uniaxial pressure is essential for understanding the pressure-dependent evolution of the structural, electronic, and magnetic properties of Heusler magnetic semiconductors.

II.4 Conclusion

In summary, hydrostatic pressure provides uniform, often enhancing effects on Heusler alloy properties across mechanical, electronic, magnetic, and optical domains, while uniaxial stress induces anisotropic structural transformations and directional tuning of electronic and optical behaviors, sometimes weakening certain properties. Both mechanisms are powerful tools for tailoring Heusler alloys for advanced applications in spintronics, shape memory devices, magnetic refrigeration, and optoelectronics

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Chapter III

Results and discussion

III.1 Introduction:

In a solid, the interactions between elementary particles, such as ions and electrons, along with the arrangement of atoms and molecules and their physical state, are fundamental in exploring the various physicochemical properties that define the complex organization of these particles. Consequently, using computational methods is vital as a complementary approach to understanding physical systems.

Simulations in this field generally depend on three main types of computational techniques:

1. Empirical Methods: These methods use experimental data to determine the values of various parameters that describe the semiconductor material.
2. Semi-Empirical Methods: These require both atomic parameters and experimental data to predict properties that have not yet been measured experimentally.
3. Ab-Initio Methods (First-Principle Methods): These rely solely on atomic constants as inputs to solve the Schrödinger equation.

In recent years, significant advancements have been made in the structural studies of atoms, molecules, and clusters across various areas. The incorporation of relativistic effects and the application of pseudopotentials for core electrons have enabled the expansion of ab-initio studies to encompass the entire periodic table. Nevertheless, some compounds still pose intricate challenges. Transition metals, characterized by their partially filled d shells and the crucial influence of electron correlation, continue to present numerous unresolved issues.

In an N-body system, addressing the Schrödinger equation necessitates specific approximations. The most significant among these are the ab-initio or "first-principles" methods, which encompass:

Hartree–Fock (HF) methods, frequently utilized by chemists.

Density Functional Theory (DFT) methods, predominantly employed by physicists.

These methods aim to solve the Schrödinger equation without incorporating parameters that are fine-tuned to experimental data; essentially, they seek to ascertain the wave function (Ψ) and the energy (E) of a quantum system.

The resolution of the Schrödinger equation for complex systems necessitates the introduction of approximations that are common to both Hartree-Fock (HF) and Density Functional Theory (DFT). Two key approximations are the Born-Oppenheimer adiabatic approximation and the orbital approximation.

The Born-Oppenheimer approximation allows us to separate electronic motion from nuclear motion, simplifying the problem. The orbital approximation further reduces an interacting many-particle system into a more manageable system of independent particles.

From these approximations, the HF method is derived, which expresses the multi-electronic wave function as a product of single-electron spin-orbital functions. In contrast, Density Functional Theory represents the electronic density of the system as a sum of the densities associated with each particle.

III.2 Computational details

The structural, electronic and magnetic properties of the studied Heusler compounds were performed using density functional theory (DFT) [2,4], within the framework of first principles calculation.

The full-potential linearized augmented plane wave (FP-LAPW) method [5,7] as implemented in the WIEN2k code [8] was employed. The generalized gradient approximation (GGA) [9] with Perdew-Burke-Ernzerhof (PBE) and the modified Becke-Johnson (mBJ) [10] potential was used to improve electronic property descriptions.

The cutoff parameter was set to $RMTK_{max} = 9$, where RMT denotes the smallest muffin-tin radius and K_{max} is the largest reciprocal lattice vector. The cutoff energy of -6.0 Ry. Brillouin zone integrations were conducted using a $14 \times 14 \times 14$ Monkhorst-Pack k-point mesh [11], with convergence criteria of 10^{-4} Ry for energy and 0.001 electrons for charge.

Phonon dispersion calculations were performed using density functional perturbation theory (DFPT) in the QUANTUM ESPRESSO package [12,18], employing ultrasoft pseudopotentials from the PSLibrary project for accurate electron-ion interaction treatment.

III.3 Part 1: Quaternary Heusler compound CoMnTaSb

III.3.1 Structural properties

Heusler alloys are ternary intermetallic compounds characterized by the general formula X_2YZ and belong to the $L2_1$ structural class (space group $Fm-3md$). The quaternary Heusler alloys $XX'YZ$, which have the space group $F-43m$, are created by replacing one of the X atoms in X_2YZ with a different transition metal element, X' . Quaternary Heusler alloys that crystallize in the LiMgPdSn structure [19] can indeed display three distinct crystal structures, commonly referred to as Type I, Type II, and Type III. For the compound being examined, the three different potential sites are as follows: (i) Type I: Co ($3/4, 3/4, 3/4$), Mn ($1/4, 1/4, 1/4$), Ta ($1/2, 1/2, 1/2$), and Sb (0, 0, 0), (ii) Type II: Co ($1/2, 1/2, 1/2$), Mn ($1/4, 1/4, 1/4$), Ta ($3/4, 3/4, 3/4$), and Sb (0, 0, 0), and (iii) Type III: Co ($3/4, 3/4, 3/4$), Mn ($1/2, 1/2, 1/2$), Ta ($1/4, 1/4, 1/4$), and Sb (0, 0, 0). To ascertain the optimal structure of the CoMnTaSb quaternary Heusler alloy, we performed calculations of total energy as a function of volume for both the non-magnetic (NM)

and ferromagnetic (FM) states across three different structures. As shown in [Figure.III.1](#), CoMnTaSb tends to crystallize in the Type I structure in the ferromagnetic (FM) state.

The Murnaghan equation of state [\[21\]](#) is employed to fit the calculated total energies as functions of volume to derive the ground-state structural properties. The equilibrium lattice constant, bulk modulus B_0 , and its pressure derivative B' for the system under study are presented in [Table.III.1](#). The ground-state structural characteristics of the CoMnTaSb compound align with theoretical findings for CoMnTaGe and CoMnTaSi [\[22\]](#).

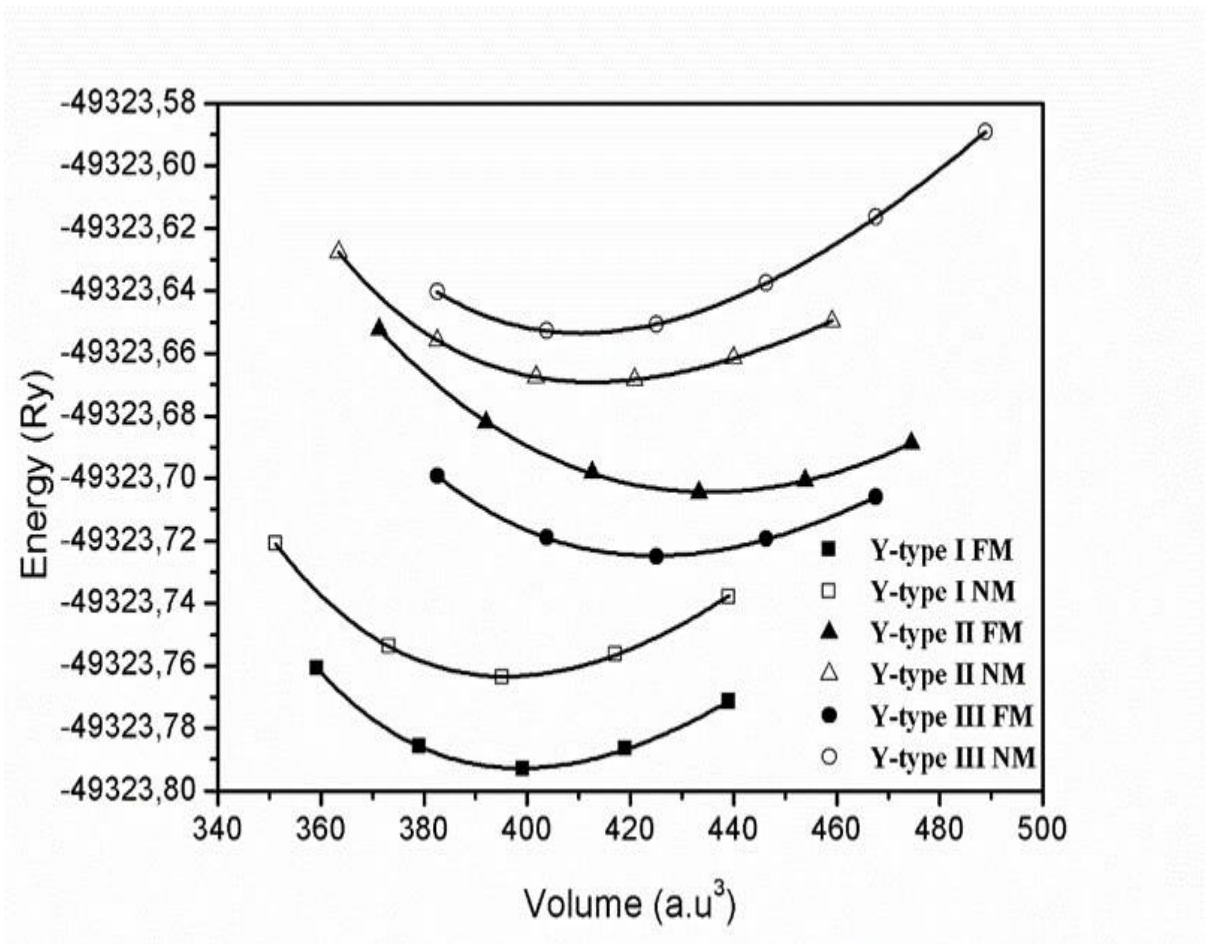


Fig.III.1. Volume optimization curve for CoMnTaSb quaternary Heusler alloy for the non-magnetic (NM) and ferromagnetic (FM) states in Y-type (I), Y-type (II) and Y-type (III) structures.

Table.III. 1. Calculated lattice constants a_0 (Å), the bulk modulus B_0 (GPa) and its pressure derivate B' , formation energy E_f (eV/atom), cohesive energies E_{coh} (eV/atom) and elastic constants C_{ij} (GPa) in the Y-type (I) structure.

Compound	a_0	B_0	B'	E_f	E_{coh}	C_{11}	C_{12}	C_{44}
CoMnTaSb	6.18	189.75	5.64	-0.44	-4.23	250.120	169.764	87.890
CoMnTaGe[20]	5.96	164.26	4.43	-0.24	/	/	/	/
CoMnTaSi[20]	5.88	244.25	5.14	-0.21	/	/	/	/

III.3.2 Stability

In this section, we examine the phase stability of the CoMnTaSb EQH compound by analyzing its mechanical and dynamical properties, cohesive and formation energies, as well as its convex hull distance. Elastic constants are used to measure a material's ability to return to its original shape after experiencing stress. For a CoMnTaSb compound with a cubic structure, the stability conditions [23] are determined by three independent elastic constants (C_{11} , C_{12} and C_{44}):

$$\begin{aligned} &C_{11} - C_{12} > 0, \quad C_{11} > 0, \quad C_{44} > 0 \quad \text{and} \\ &\{C_{11} + 2C_{12} > 0 \quad \text{and} \quad (1) \\ &C_{12} < B < C_{11} \end{aligned}$$

The corresponding values of C_{ij} constants listed in Table. III. 1 reflects the mechanical stability of the material under investigation, fulfilling all outlined criteria.

The phonon dispersion curves along the W-L- Γ -X-W-K directions in the Brillouin zone displayed in Figure. III. 2 indicate the dynamical stability of the anticipated EQH compound, as evidenced by the lack of imaginary frequencies.

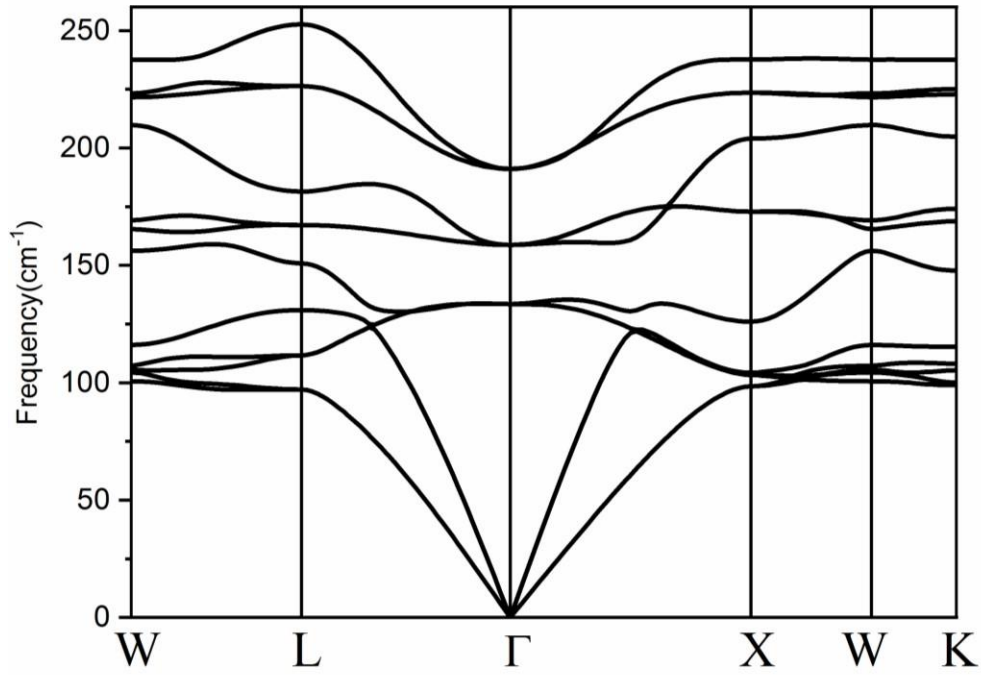


Fig.III.2. Calculated phonon dispersion curves for CoMnTaSb alloy along lines of high symmetry in the Brillouin zone.

The formation energy is calculated via the expression according to:

$$E_f = E_{Total}^{CoMnTaSb} - (E_{Co}^{bulk} + E_{Ta}^{bulk} + E_{Mn}^{bulk} + E_{Sb}^{bulk}) \quad (2)$$

And the cohesive energy is calculated using the formula:

$$E_{coh} = (E_{Co}^{iso} + E_{Ta}^{iso} + E_{Mn}^{iso} + E_{Sb}^{iso}) - E_{Total}^{CoMnTaSb} \quad (3)$$

Where $E_{Total}^{CoMnTaSb}$ is the equilibrium total energy of the CoMnTaSb, E_Z^{bulk}

and E_Z^{iso} correspond to the total energy per atom of each element in the bulk and the energy of the isolated Z atom, respectively. The calculated values of E_f and E_{coh} summarized in [Table. III. 1](#) suggests that the CoMnTaSb compound is energetically stable and feasible for experimental synthesis. Furthermore, the predicted formation energy of the CoMnTaSb compound is lower than that of the CoMnTaGe and CoMnTaSi compounds, indicates a higher level of thermodynamic stability [\[21\]](#).

The Curie temperature T_C of this alloy have also been determined using the equation [\[24, 25\]](#):

$$T_c = \frac{\Delta E}{3k_B} \quad (4)$$

Where ΔE is the total energy difference between the ferromagnetic and non-magnetic states and k_B is the Boltzmann constant. This alloy is a promising spintronic material due to its high Curie temperature around 1545.43 K.

Another important parameter in the investigation of the thermodynamic stability of materials and compounds is the convex hull distance, given by [26, 27]:

$$E_{HD} = E_f - E_{hull} \quad (5)$$

where E_{hull} is the energy of the convex hull, defined as the sum of the formation energies of the constituent elements (the stable phases in which the substance under study decomposes) multiplied by the relative phase compositions [28-31].

By definition, a thermodynamically stable compound lies on the convex hull, i.e., $E_f \leq E_{hull}$. According to the Open Quantum Materials Database (OQMD) [32, 33], the CoMnTaSb compound decomposes into $Ta_4Co_5Sb_5$, Mn, and $TaMn_2$. By applying equation (3) in conjunction with the full-potential linearized augmented plane waves (FP-LAPW) method, we have determined a convex hull distance value of -0.03046 eV/atom. This finding strongly suggests that the CoMnTaSb compound is indeed thermodynamically stable.

Nevertheless, our computed elastic constants, phonon spectra, cohesive and formation energies, along with convex hull distance suggest stability of our compound and its appropriation for experimental synthesis.

III.3.3 Electronic and magnetic properties

Band structure calculations of the equiatomic quaternary Heusler (EQH) compound CoMnTaSb were performed using the generalized gradient approximation (GGA) and a combination of

GGA and modified Becke-Johnson potential (mBJ). Results are shown in [Figure. III. 3](#), There exists a notable distinction between the band energies of the majority (spin-up) and minority (spin-down) states, which contributes to the emergence of an indirect band gap near the Fermi level in both the spin-down and spin-up channels. This phenomenon results in a semiconductor character for both spin states. The band gaps are approximately 0.189 eV and 0.441 eV along the Γ -X symmetry direction, as determined by GGA and GGA + mBJ, respectively, in the context of the spin-up state.

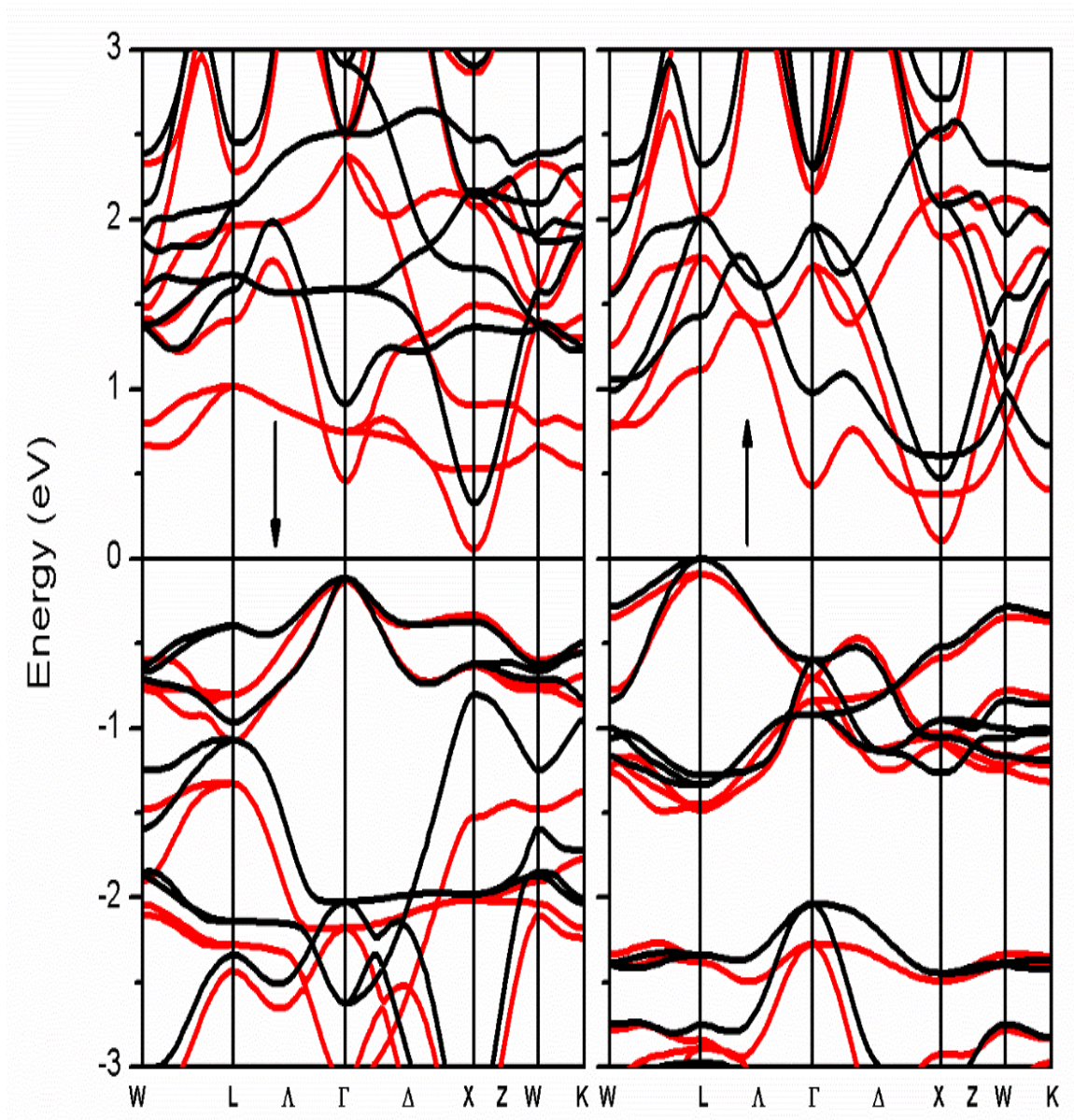


Fig.III.3. Calculated band structures of the quaternary Heusler compound CoMnTaSb obtained from GGA (red line) and GGA + mBJ (black line).

In the case of the spin-up channel, the energy gaps calculated using GGA and GGA + mBJ are roughly 0.196 eV and 0.470 eV along the L-X direction, respectively. It is important to emphasize that, for the spin-up channel, the valence band maximum (VBM) identified by GGA + mBJ coincides with the Fermi level at the L point.

The difference in the symmetry directions and the energy gap values between the spin-up and spin-down channels indicates that the mechanisms controlling these two spin orientations are different. [34,36].

To perform a more comprehensive analysis of the electronic properties of the CoMnTaSb compound, [Figure. III. 4](#) displays the total density of states (TDOS) alongside the partial density of states (PDOS). The density of states profiles obtained from the GGA and GGA + mBJ methods for the CoMnTaSb compound show significant similarities. The TDOS reveals that both majority and minority spin states demonstrate semiconducting characteristics, which is consistent with the results from the band structure calculations. The valence band in both spin-up and spin-down channels is predominantly composed of Mn-3d and Co-3d states, with neglected contributions from Ta and Sb atoms ranging from -2 and 0 eV. In the spin-up state, it is the Mn-deg and Co-deg electrons that contribute the most to the valence band. Conversely, in the spin-down state, the primary contribution duo to the Mn-dt2g and Co-dt2g electrons.

Ranging from 0 to 2 eV. In the spin-up channel, the conduction band is primarily governed by the Mn-3d states, with a secondary contribution from the Ta-3d states, where the Mn-deg orbitals play the dominant role. The Co atom, however, contributes negligibly in this channel. Conversely, in the spin-down channel, the major contributions originate from Mn-deg and Co-

deg states. At the Fermi level, a distinct difference is observed in the relative contributions of the atomic states to the conduction and valence bands across the two spin channels. This behavior is consistent with the findings reported by Liu et al. for CoTiFeAs [37].

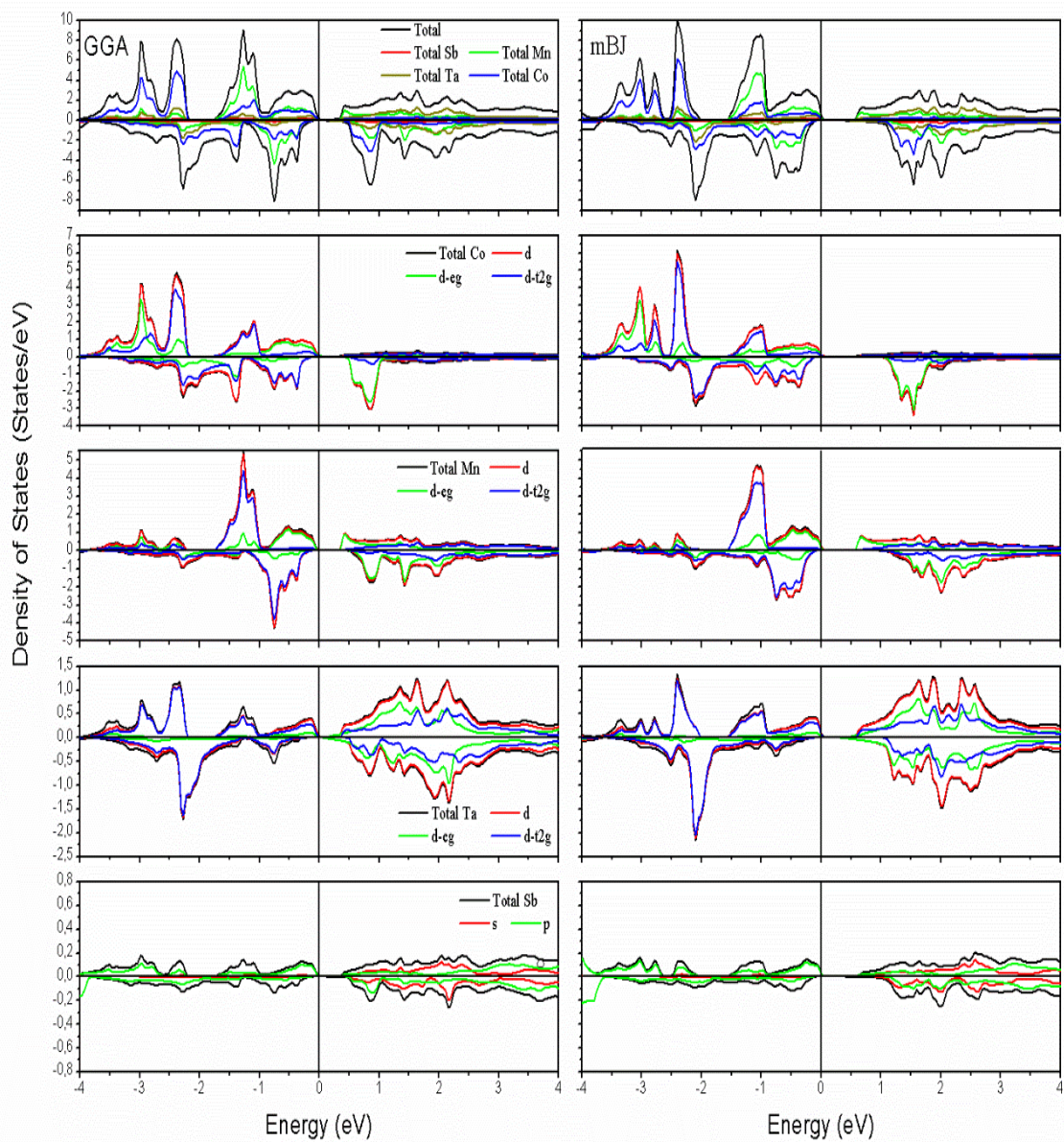


Fig.III.4. total (TDOS) and partial (PDOS) densities of states calculated using GGA and GGA + mBJ

Heusler alloys Orbital hybridization has been extensively explored through ab-initio studies [26, 37–40]. In addition to the conventional d–d hybridization, the interaction between the sp-element and transition-metal atoms plays a crucial role. Results, both the structural stability of the alloy and the emergence of the band gap that are strongly influenced by the combined effects of p–d and d–d hybridizations.

Özdoğan et al. [41] examined the orbital hybridization of many quaternary Heusler. Allowed as to explore the origin of the band gaps in the magnetic semiconductor CoMnTaSb that is the energy gap present within the majority band is attributed to the CoMn-2e_u and CoMnTa-2e_g states, while in the minority band, the Fermi level (E_F) is situated between the CoMn-3t_{1u} and CoMn-2e_u orbitals.

Table. III. 2 lists the calculated total and atomic magnetic moments. CoMnTaSb has 26 valence electrons (Z) and a total magnetic moment per formula unit of $m_{\text{tot}} = 2.00 \mu_B$, which follow the Slater-Pauling rule $m_{\text{tot}} = (Z - 24) \mu_B$. while the Heusler alloys CoMnTaGe and CoMnTaSi, has 25 valence electrons per unit cell, were found to have a total magnetic moment of $1 \mu_B$ [20].

The total magnetic moment is originally dominated by Co atom, while the Mn atom provides the next significant contribution. In contrast, with a neglected contribution of Ta and Sb atoms. As presented in Table 2, the magnetic moments of Co and Mn display an antiferromagnetic interaction with that of Ta. This observation is consistent with results reported in previous studies [22].

Table.III. 2. Total magnetic moment m_{tot} (μ_B), individual magnetic moments m_X (μ_B) ($X = \text{Co, Mn, Ta, Sb}$) and interstitial magnetic moment m_{Inter} (μ_B) of CoMnTaSb Heusler compounds.

Compound	method	$m_Z (\mu_B)$	$m_{Co}(\mu_B)$	$m_{Mn}(\mu_B)$	$m_{Ta}(\mu_B)$	$m_{Inert}(\mu_B)$	$m_{tot}(\mu_B)$
CoMnTaSb	GGA	0.011	1.233	0.840	-0.040	-0.044	2.00
	mBJ	0.016	1.428	0.789	-0.082	-0.146	2.00
CoMnTaGe[20]	GGA	0.004	0.703	0.364	-0.016	-0.028	1.00
CoMnTaSi[20]		-0.002	0.615	0.532	-0.060	-0.048	1.00

III.3.4 Hydrostatic pressure effect

In this section, we have assessed the electromagnetic characteristics under hydrostatic pressure, as well as their mechanical and dynamic stability.

The composite's stability during high-pressure conditions cannot be overstated so [Figure. III. 5](#) depicts the phonon dispersion spectra and verifies the dynamic stability of our compound, alongside [Table. III. 3](#), which presents the calculated Cij constants at different strains from 2 to 10 GPa. This further affirms the mechanical stability.

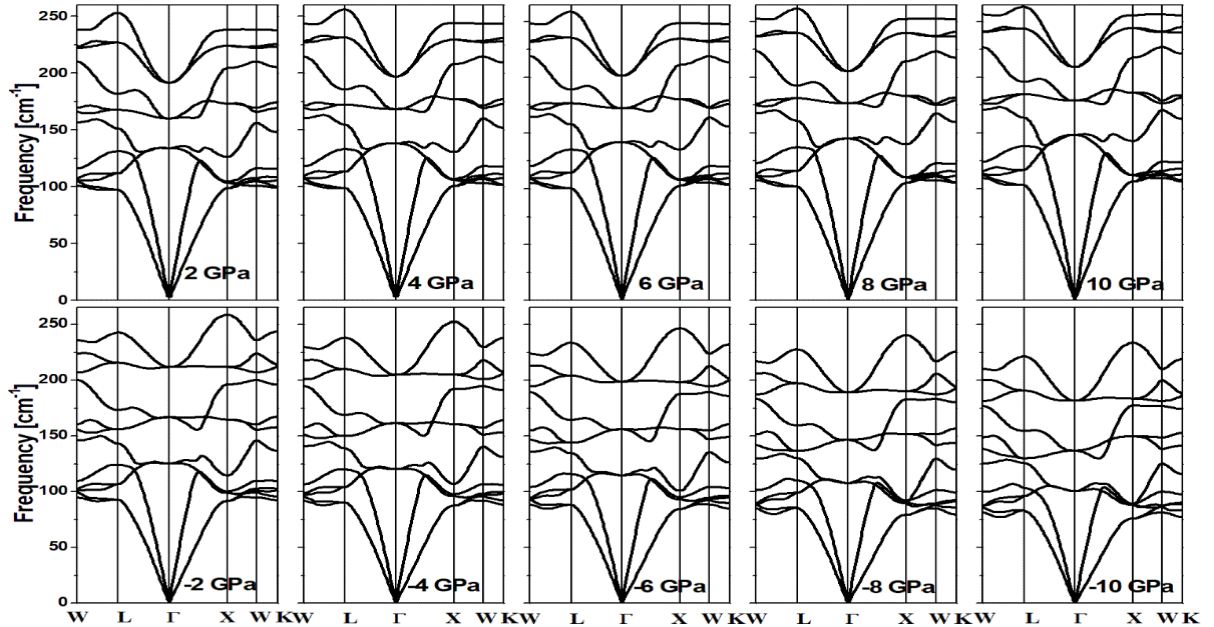


Fig.III.5. Computed phonon dispersion spectra of CoMnTaSb under hydrostatic pressure

Table. III. 3. Calculated elastic constants C_{ij} (GPa) of CoMnTaSb under hydrostatic pressure.

Pressure (GPa)	Lattice constants (Å)	C_{11}	C_{12}	C_{44}
10	6.08824	284.9939	213.9351	106.2317
8	6.10514	296.1248	199.8214	105.6905
6	6.12293	293.0132	186.8377	101.8346
4	6.14169	274.8427	182.6159	93.9218
2	6.16154	273.1977	175.739	98.4967
0	6.1847	250.1206	169.7643	87.8908
-2	6.20503	224.8098	167.6387	75.3704
-4	6.22902	209.1463	163.8092	66.0051
-6	6.25479	214.9427	147.6649	76.0403
-8	6.28262	215.8493	132.6953	76.7532
-10	6.31284	183.1921	133.8415	47.9798

The CoMnTaSb compound's electrical properties were deduced using the mBJ potential to calculate their spin-resolved band structure under hydrostatic pressure varying from -10 to 10 GPa, covering the lattice parameter interval between 6.088 to 6.313 Å. Under the defined negative and positive pressures, the semiconducting behavior remains consistent, keeping the same band gap directions at L-X for the spin-up states and at Γ -X for the spin-down states.

The conduction band minimum (CBM) and the valence band maximum (VBM) positions are illustrated in [Figure. III. 6](#). Both the conduction band minimum (CBM) and the valence band maximum (VBM) experience an upward shift, leading to a gradual widening of the band gap as pressure increases in the spin-down channel. In contrast, in the spin-up channel, the VBM consistently remains at 0 eV throughout the entire pressure range [\[42\]](#). The CBM responds more strongly to pressure than the VBM. Apart for -10 GPa consistently narrows

with rising pressure.

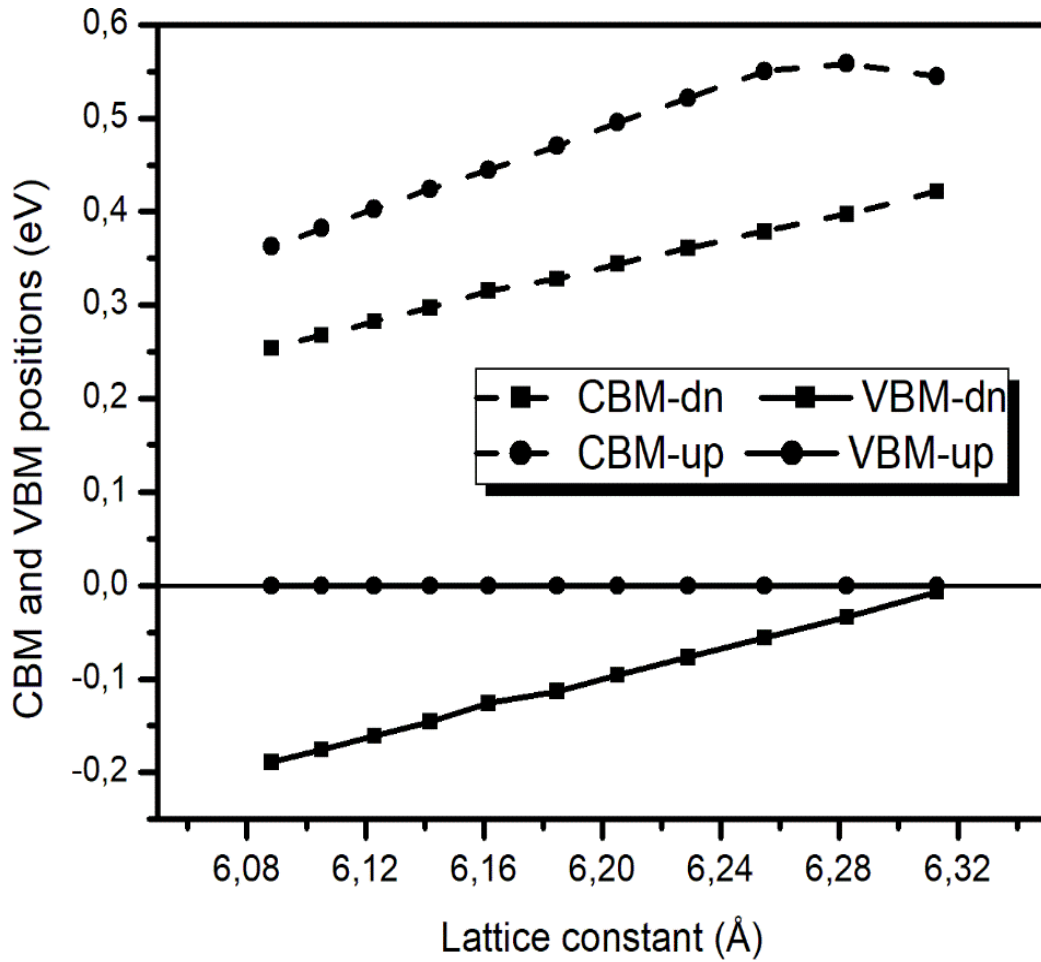


Fig. III.6. Conduction band minimum (CBM) and valence band maximum (VBM) positions computed for various lattice parameters of CoMnTaSb.

Figure. III. 7 presents the pressure dependence of both the band gaps in the two spins channels and the lattice parameter. Under compression, the band gap in the spin-down channel exhibits a steady increase, whereas the spin-up channel displays a distinct trend: it first widens slightly before undergoing a rapid reduction. These findings agree with those of Zhou et al. [43] for Mn₂CoAl Heusler alloys, where the spin-up band gap was reported to increase continuously with pressure. In their study, the spin-down band gap expanded with increasing pressure up to 8.0 GPa, however, beyond it became gapless up to 38.0 GPa.

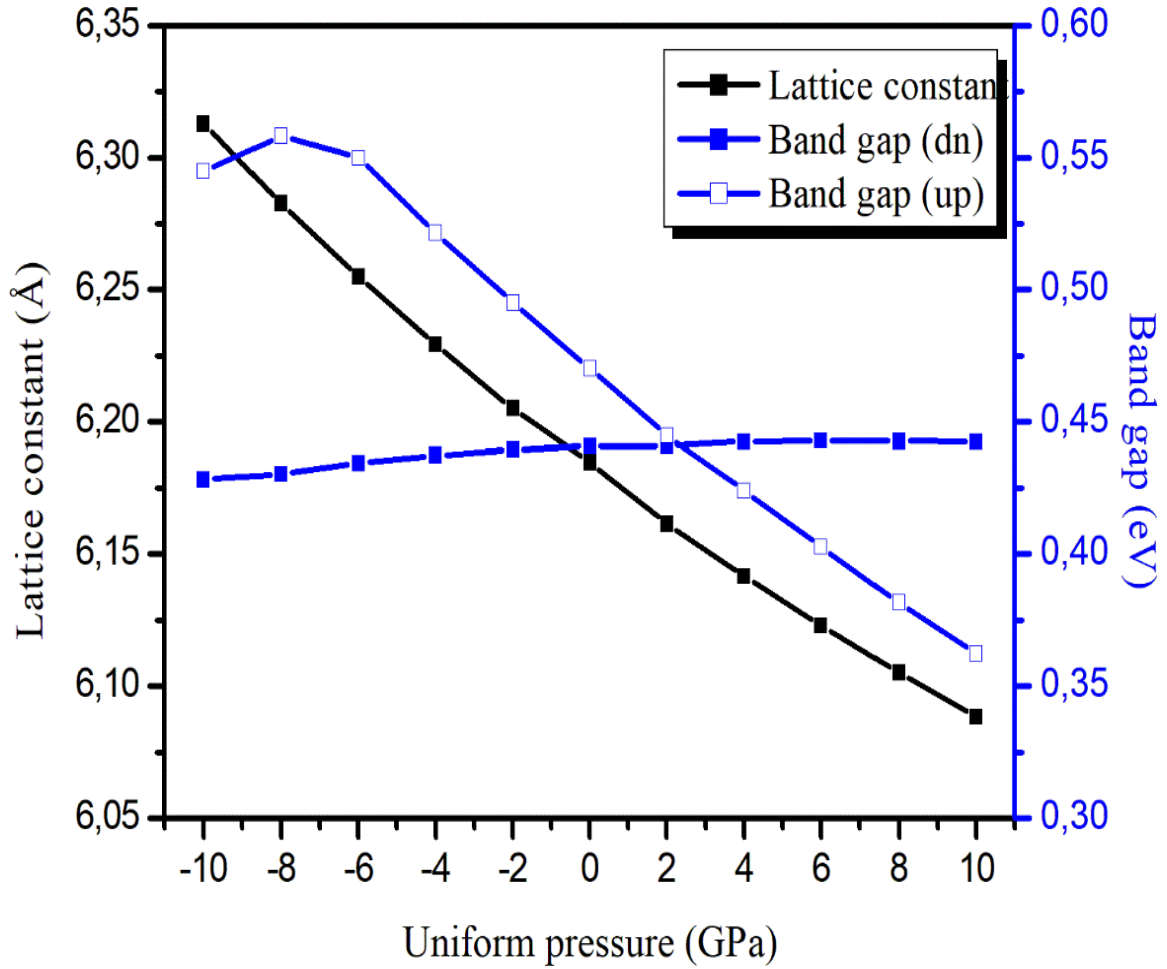


Fig.III.7. Variation of the band gaps in the two spin channels and the lattice parameter as a function of pressure.

To conclude, the variation of the total and individual atomic magnetic moments on the lattice constants of the CoMnTaSb Heusler compound was examined with respect to the lattice constant and is shown in [Figure. III. 8](#). Over the entire pressure interval, a constant value $2 \mu_B$ is noted for the total magnetic moment. In contrast, the atomic contributions display variant trends: the magnetic moments of Co and Mn diminish steadily, whereas the Ta and the Sb moments rise gradually.

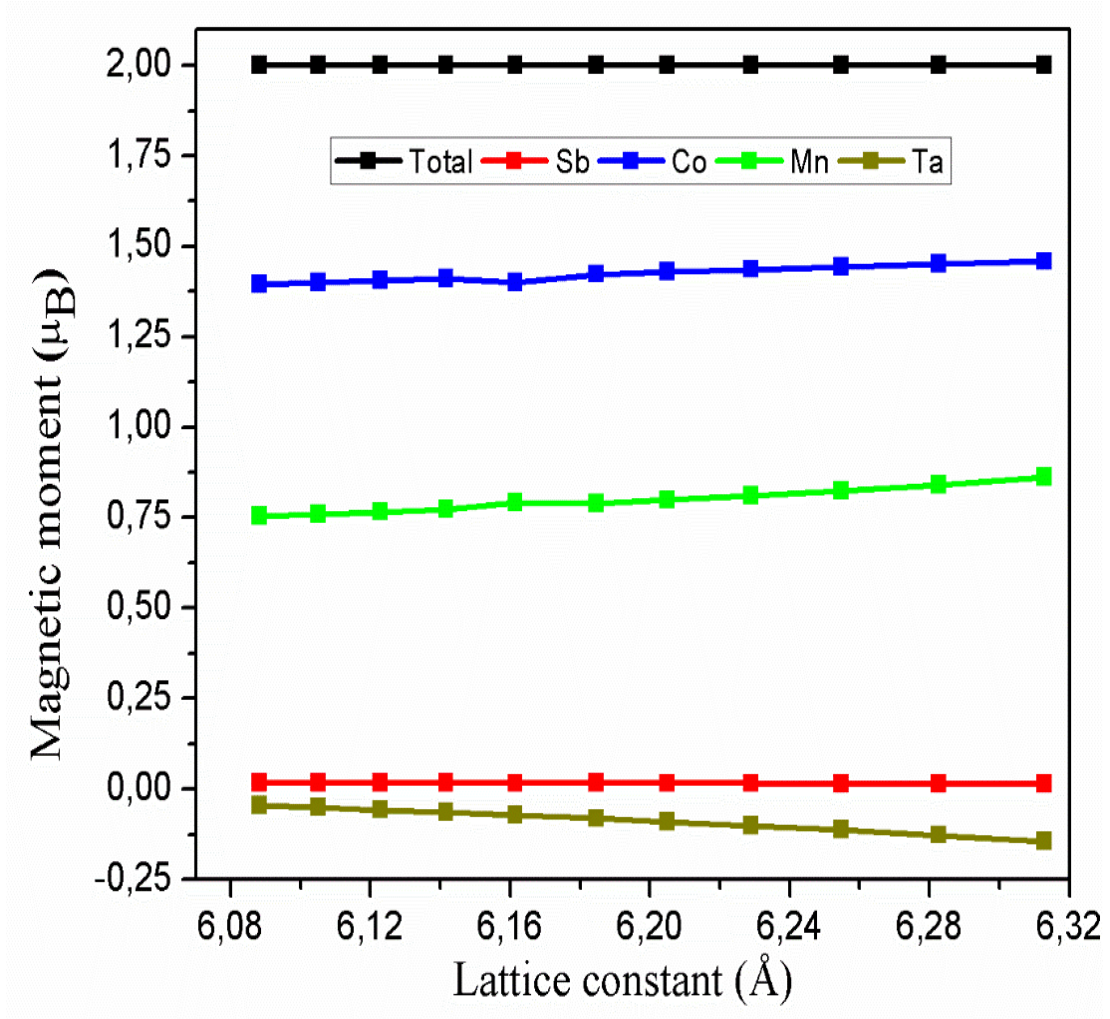


Fig. III.8. Variation of the total and atomic magnetic moments as a function of the lattice parameter.

III.3.5 Uniaxial effect

Uniaxial pressure has been applied on the electronic and magnetic properties of the CoMnTaSb compound, we computed the spin-resolved band structure corresponding for pressures ranging from 2 to 10 GPa within the GGA approach. The semiconductor characteristics in both spin states are maintained under the specified pressures from 2 to 6 GPa. At 8.0 GPa the band gap value is set as 0.097 in spin down direction with a gapless value for the spin up direction leading to a half metallic behavior, at 10 GPa a gapless value for both spin directions resulting a metallic

character. The directions of the band gaps are unaffected; they occur at Δ -N for the spin-up states and at Γ -N for the spin-down states.

Figure.III.9. illustrates the band gap evolution in both spin channels as a function of pressure. As pressure increases, the band gap in the spin-down channel initially increases rapidly but then decreases gradually. In contrast, the spin-up channel exhibits different behavior: the band gap decreases from 0 to 2 GPa and from 6 to 8 GPa, with a temporary stability observed between 2 and 6 GPa. Ultimately, the spin-up channel becomes gapless beyond 8.0 GPa.

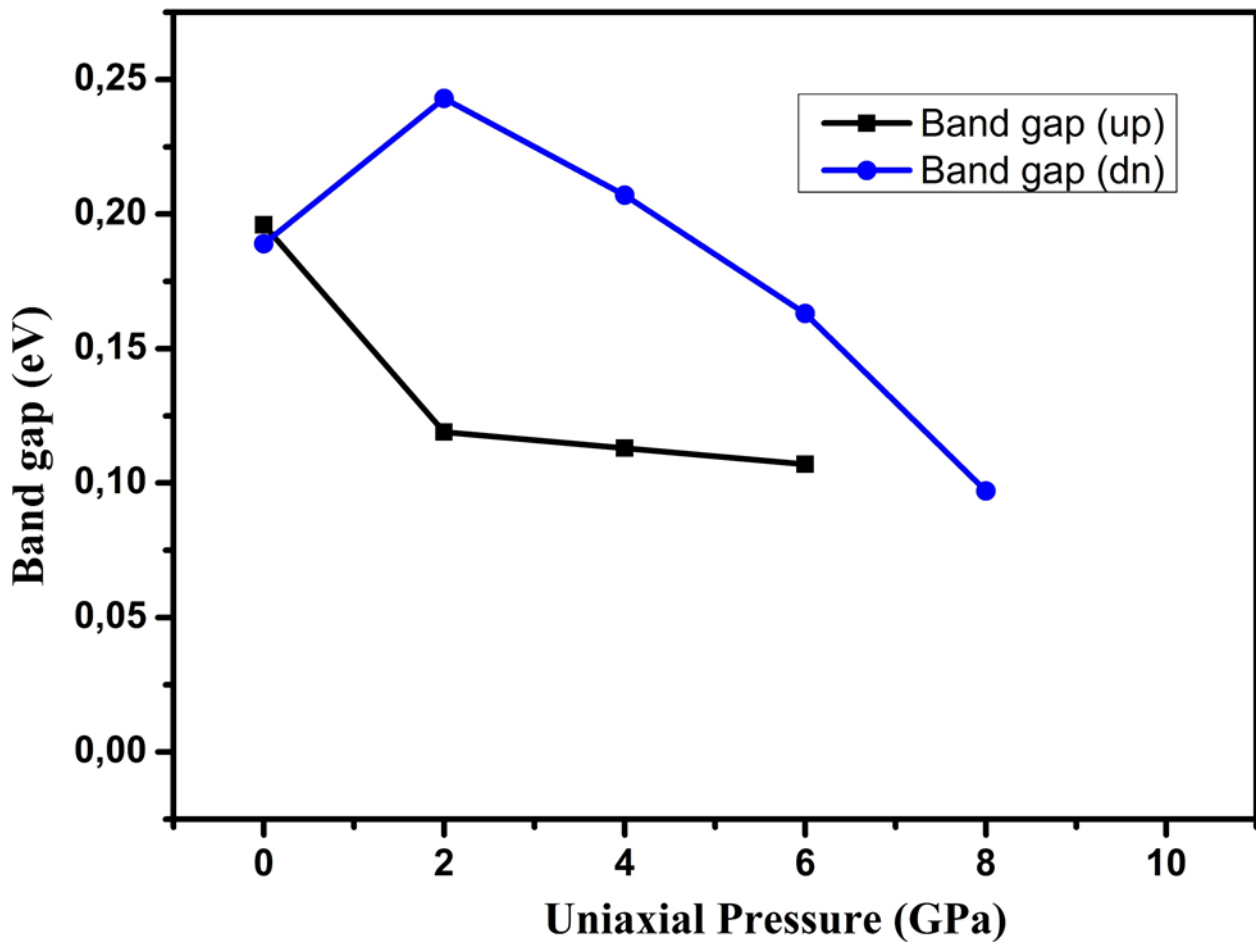


Fig.III.9. Variation of the band gaps in the two spin channels as a function of uniaxial pressure.

Finally, we investigated the dependence of the total and individual atomic magnetic moments under uniaxial pressure ranging from 2 to 10 GPa of the CoMnTaSb Heusler compound. As summarized in [Figure.III.10](#), the total magnetic moment values remain constant across the range of applied pressures; consistently equal to 2 μ_B . While the magnetic moments of Co atoms gradually decrease, Mn and Sb atom's magnetic moment gradually increases, while Ta atom's magnetic moment decreases at a slower rate.

Table. III. 4. Calculated lattice constants a_0 (Å) and c (Å), and bang gap Energy E_g for both spin directions.

CoMnTaSb	a	c	Eg up	Eg dn
0	6.18	6.18	0.196	0.189
2	4.40	6.09	0.119	0.243
4	4.44	5.94	0.113	0.207
6	4.48	5.81	0.107	0.163
8	4.52	5.69	/	0.097
10	4.55	5.56	/	/

Table. III. 5. Total magnetic moment m_{tot} (μ_B), individual magnetic moments m_X (μ_B) ($X =$ Co, Mn, Ta, Sb) and interstitial magnetic moment m_{Inter} (μ_B) of CoMnTaSb Heusler compounds under uniaxial pressure.

Pressure	$m_{tot}(\mu_B)$	$m_Z(\mu_B)$	$m_{Mn}(\mu_B)$	$m_{Ta}(\mu_B)$	$m_{Co}(\mu_B)$	$m_{Inert}(\mu_B)$
0	2	0.01224	0.84	-0.04	1.233	-0.044
2	2.00184	0.01224	0.83732	-0.03454	1.22559	-0.03876
4	1.99921	0.01212	0.84962	-0.03469	1.20728	-0.0351
6	2.002	0.01431	0.86813	-0.03394	1.17912	-0.02562
8	2.00127	0.01548	0.89795	-0.03634	1.14138	-0.0172
10	1.99194	0.01613	0.93723	-0.0434	1.09277	-0.0108

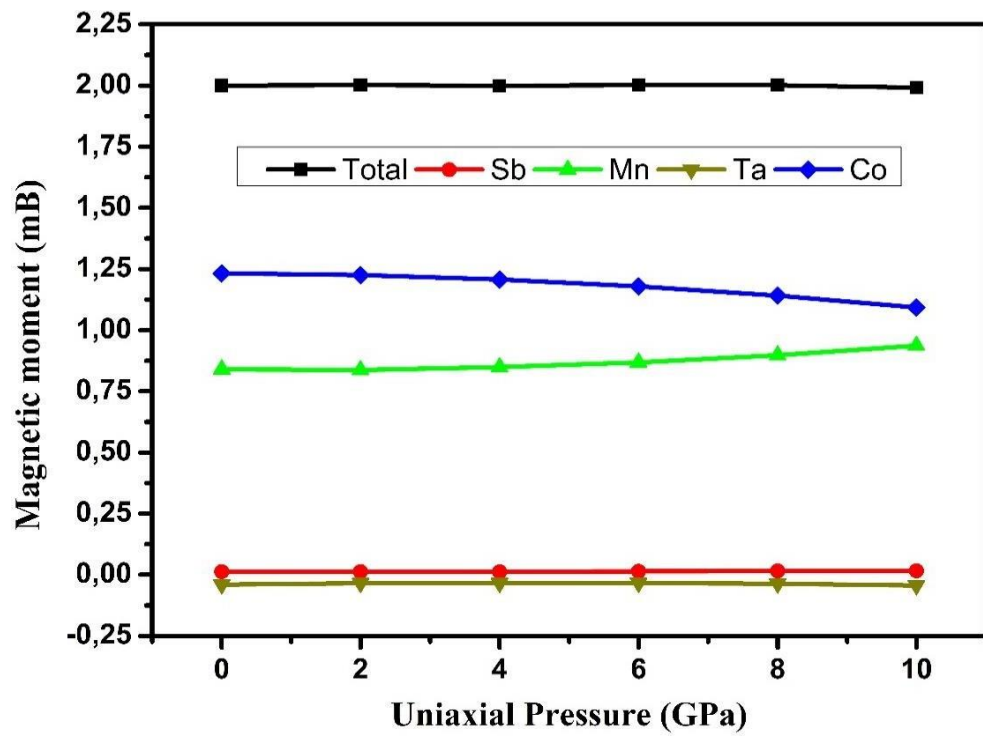
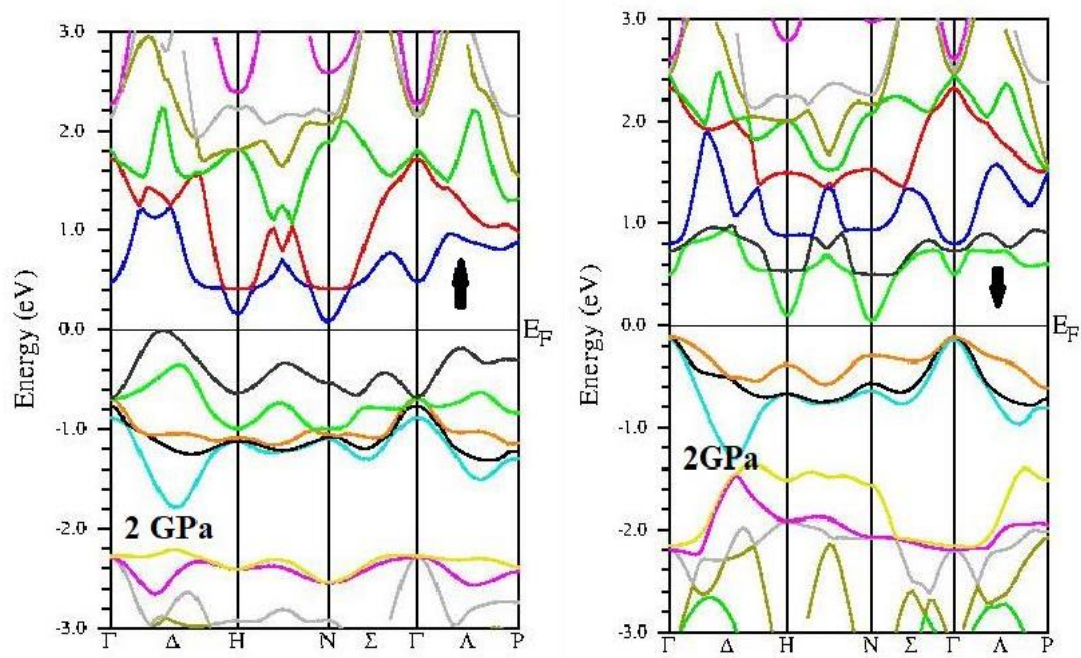
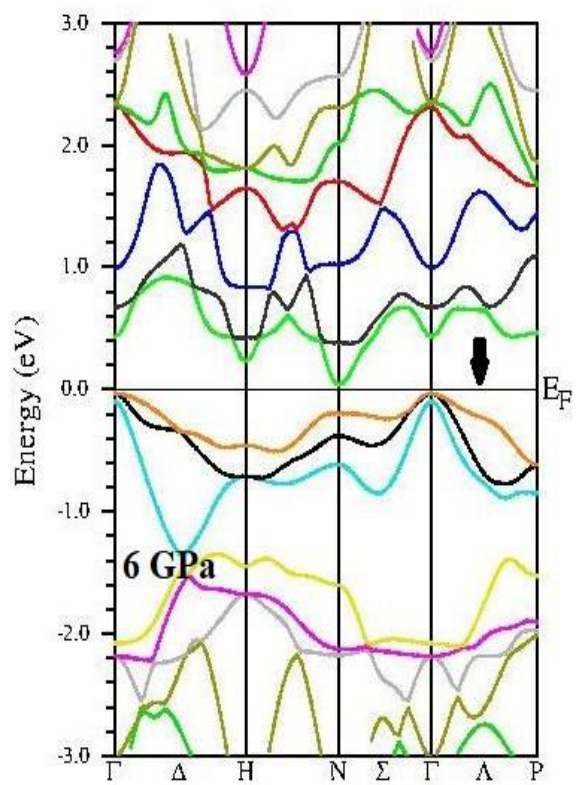
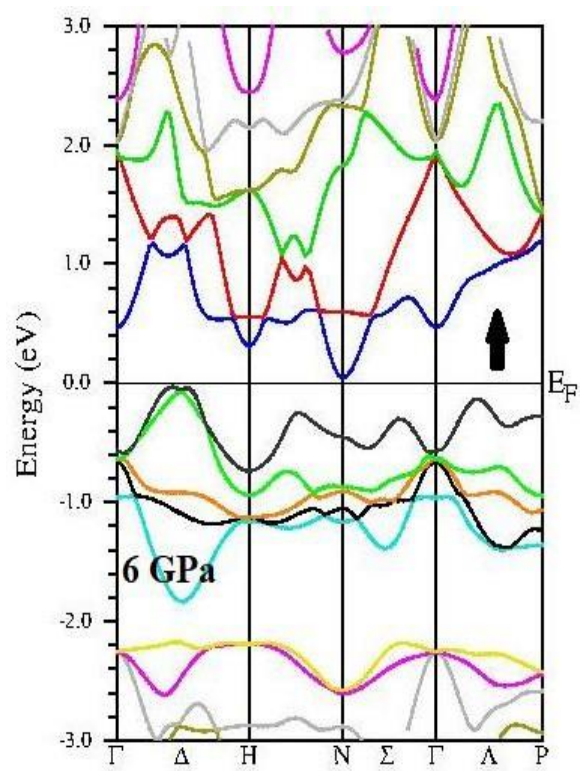
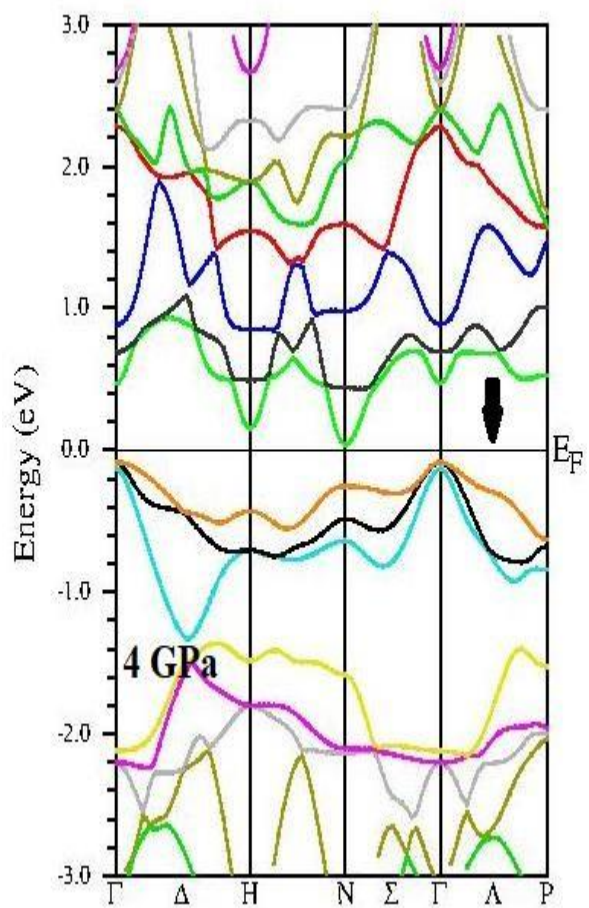
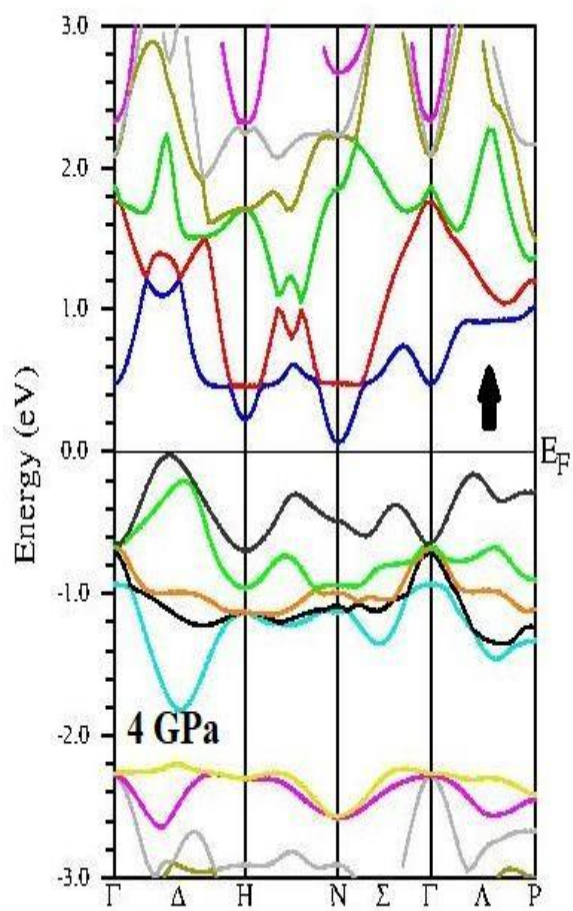


Fig.III.10. Variation of the total and atomic magnetic moments as a function of the uniaxial pressure.





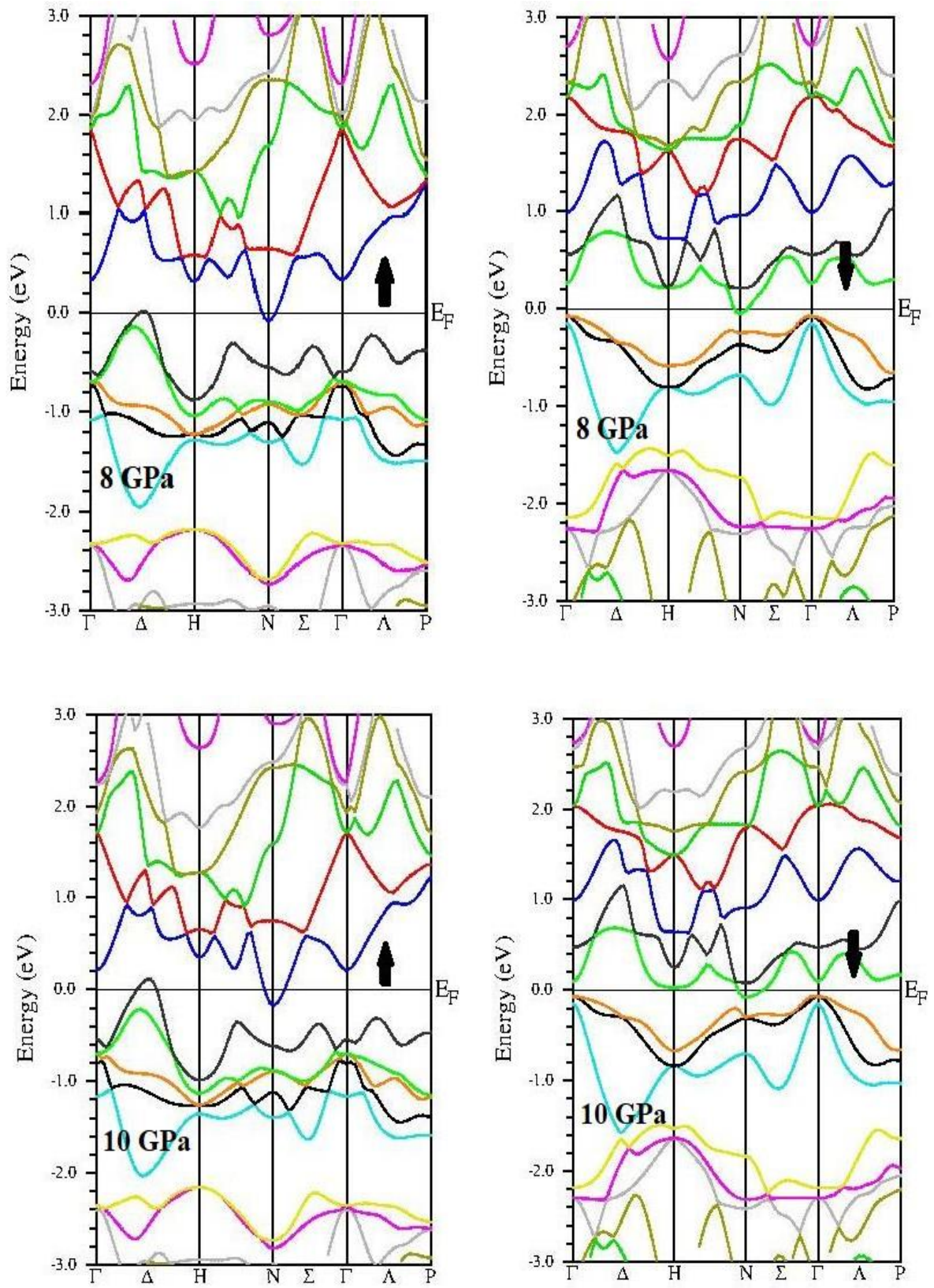


Fig.III.11. Calculated band structures of the quaternary Heusler compound CoMnTaSb obtained from GGA under uniaxial pressure.

III.4 Part 2: Full Heusler compounds Rb_2TiZ

III.4.1 Structural properties and stability:

Full Heusler Alloys, defined by the general formula of X_2YZ , can crystallize into two distinct non-equivalent structural forms: the cubic Cu_2MnAl -type phase with space group $\text{Fm}\bar{3}\text{m}$ (225) and the Hg_2CuTi -type phase with space group $\text{F}\bar{4}3\text{m}$ (216) [44,45]. In the Cu_2MnAl -type structure, the X atoms are located at the coordinates (0,0,0) and (1/2,1/2,1/2), whereas the Y and Z atoms are located at (1/4,1/4,1/4) and (3/4,3/4,3/4) respectively. In Hg_2CuTi -type structure, the coordinates (0,0,0) and (1/4,1/4,1/4) are occupied by the X atoms, while the Y and Z atoms occupy the coordinates (1/2,1/2,1/2), and (3/4,3/4,3/4), respectively. To identify the structural parameters that correspond to the most stable configuration of the Rb_2TiZ ($\text{Z} = \text{Si, Ge, Sn and Sb}$) Heusler alloys, the total energy was computed as a function of volume [46] for each of the two atomic arrangements for the ferromagnetic (FM) and non-magnetic (NM) phases across the two possible atomic arrangements. As shown in Figure. III. 12, the FM Hg_2CuTi -type structure has the lowest total energy, suggesting that it represents the most energetically favorable configuration for all the compounds studied. Table. III 6 summarizes the obtained results, namely the optimized lattice parameter, bulk modulus B_0 , and its pressure derivative B' of Rb_2TiZ ($\text{Z} = \text{Si, Ge, Sn and Sb}$).

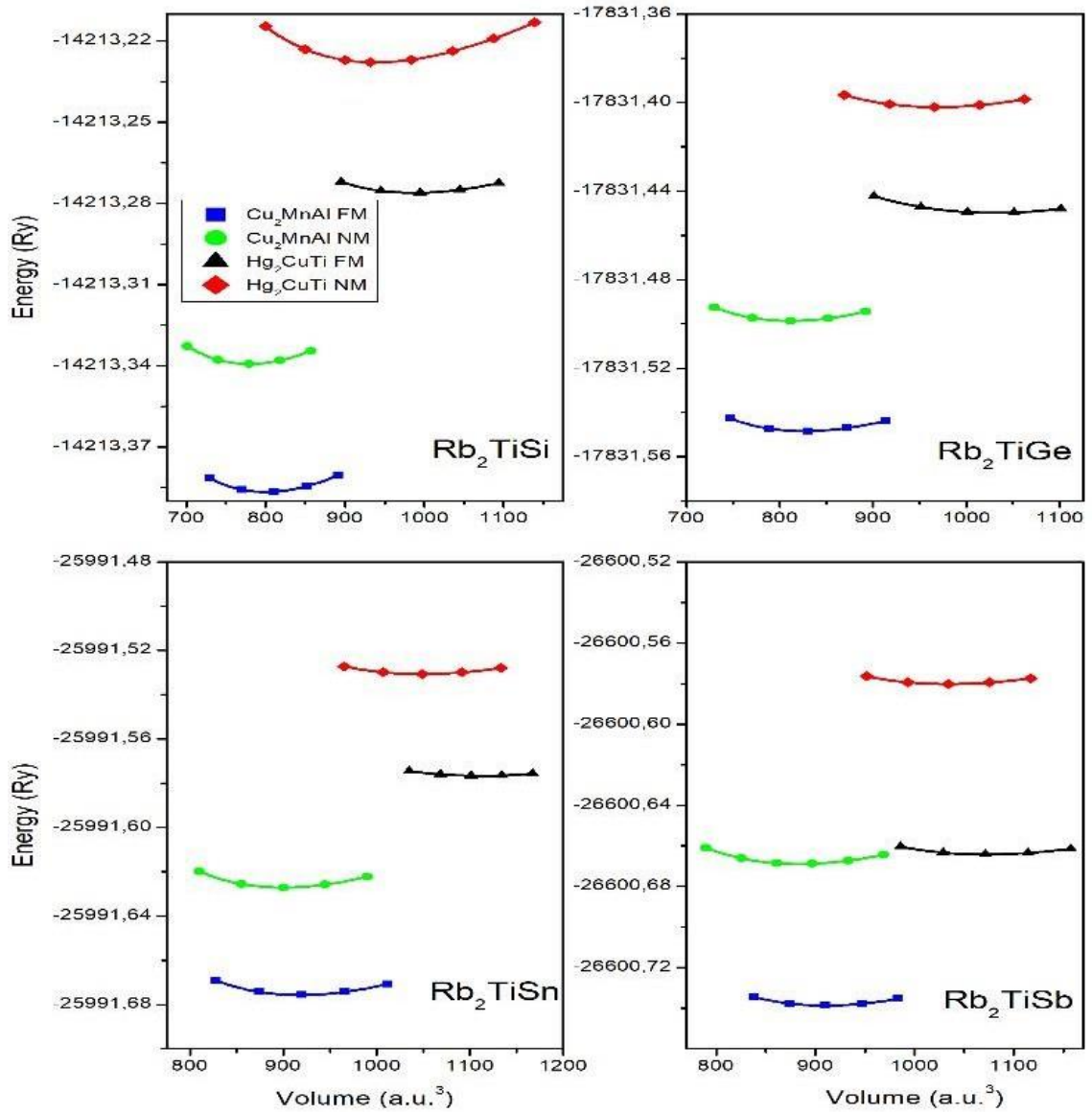


Fig.III.12. Total energy as a function of volume of Rb₂TiZ (Z = Si, Ge, Sn and Sb) compounds.

Table.III.6 The optimized lattice parameters a_0 (Å) of Rb₂TiZ (Z = Si, Ge, Sn and Sb) alloys in magnetic (FM) state of Hg₂CuTi structure, and the bulk modulus B_0 (GPa), its pressure derivate B' and total energies E_0 (Ry) per formula unit.

Compounds	Rb ₂ TiSi	Rb ₂ TiGe	Rb ₂ TiSn	Rb ₂ TiSb
Lattice constant, a_0	7.797	7.896	8.170	8.140
Bulk modulus, B_0	20.637	18.390	18.232	19.270
Derivative of B_0 , B'	4.499	4.432	4.438	4.515
Total energy, E_0	-14213.386	-17831.548	-25991.674	-26600.737

To assess the thermodynamic, mechanical, and dynamic stability of the proposed compounds, we evaluated their formation and cohesive energies, elastic constants, and phonon dispersion curves.

Table.III.7 lists the computed formation (E_f) and cohesive (E_c) energies of Rb_2TiZ ($Z = Si, Ge, Sn$, and Sb) compounds, calculated using the following formulas as mentioned in part one [47].

$$E_f = E_{Total}^{Rb_2TiZ} - (2E_{Rb}^{bulk} + E_{Ti}^{bulk} + E_Z^{bulk}) \quad (1)$$

$$E_c = E_{Total}^{Rb_2TiZ} - (2E_{Rb}^{iso} + E_{Ti}^{iso} + E_Z^{iso}) \quad (2)$$

Where $E_{Total}^{Rb_2TiZ}$ is the equilibrium total energy of Rb_2TiZ ($Z = Si, Ge, Sn$ and Sb) compounds, and E_Z^{bulk} and E_Z^{iso} are the total energies in bulk structure and in free states of the Z atom. Moreover, the formation energy of any alloy represents the energy required to decompose it into its constituent elements, whereas the cohesive energy reflects the strength of the interatomic bonds that hold these atoms together. The negative values of the formation and cohesive energies of Rb_2TiZ ($Z = Si, Ge, Sn$ and Sb) compounds indicate that these alloys possess good chemical stability and remain structurally stable in the FM Hg_2CuTi type ground state.

Table.III.7 the computed formation E_f (eV), cohesive E_c (eV) and band gap energies E_g (eV) of Rb_2TiZ ($Z = Si, Ge, Sn$, and Sb) compounds.

Compounds	E_f	E_{coh}	E_g			
			GGA		mBJ	
			up	dn	up	dn
Rb_2TiSi	-2.83	-8.39	0.135	0.836	1.133	1.248
Rb_2TiGe	-2.48	-7.99	-	0.482	0.922	1.022
Rb_2TiSn	-2.13	-7.86	0.077	0.801	1.068	1.180
Rb_2TiSb	-1.43	-8.19	-	-	0.024	2.184

To further confirm the mechanical stability of these compounds, theoretical calculations for the elastic constants were also performed.

The independent elastic constants that adequately describe the elastic behavior of the Rb_2TiZ ($Z = \text{Si, Ge, Sn and Sb}$) Heusler alloys are C_{11} , C_{12} , and C_{44} . These constants were determined by applying isotropic stress, as well as volume-conserving tetragonal and rhombohedral strains [48].

If the elastic constants C_{ij} obey the Born-Huang conditions [23], the material is considered stable. The stability criteria are given by:

$$\begin{cases} C_{11} - C_{12} > 0, C_{11} > 0, C_{44} > 0 \text{ and} \\ C_{11} > C_{12}, C_{11} + 2C_{12} > 0 \text{ and} \\ C_{12} < B < C_{11} \end{cases} \quad (3)$$

The mechanical stability of our compounds, as indicated in Table. III.8, is supported by the computed C_{ij} values that satisfy the conditions in the above equations.

Mechanical parameters of the materials, including tensile strength, brittleness, bulk modulus (B), shear modulus (G), Poisson's ratio (ν), Young's modulus (Y), and elastic anisotropy factor (A), can be derived from the following equations [49-51]:

$$B = \frac{C_{11} + 2C_{12}}{3} \quad (4)$$

$$G = \frac{1}{5}(3C_{44} + C_{11} - C_{12}) \quad (5)$$

$$Y = \frac{9BG}{3B + G} \quad (6)$$

$$\nu = \frac{1}{2} \left(1 - \frac{E}{3B} \right) \quad (7)$$

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (8)$$

$$C_p = C_{12} - C_{44} \quad (9)$$

The values of the bulk modulus for Rb_2TiZ ($Z = \text{Si, Ge, Sn and Sb}$) are comparable, suggesting that these compounds exhibit comparable resistance to compression. They are within the range of values derived from Murnaghan's equation of state.

To differentiate between brittle and ductile materials, the Pugh ratio B/G [44-54] is used.

According to Pugh's criterion, a compound is classified as brittle when its bulk-to-shear modulus ratio (B/G) is less than 1.75, and as ductile when this ratio exceeds 1.75. The calculated B/G values for Rb_2TiSi , Rb_2TiGe , Rb_2TiSn , and Rb_2TiSb are 1.240, 1.256, 1.284, and 1.454, respectively, indicating that all these compounds exhibit a brittle character. The Poisson's ratio (ν) [55] and Cauchy pressure (C_p) [56,57] given by $(C_{12} - C_{44})$, can be used to assess the brittleness or ductility of a material. When the Poisson ratio falls below the critical threshold of 0.26, the material is deemed brittle; conversely, it is classified as ductile if it exceeds this value. Furthermore, a material exhibiting a negative (or positive) Cauchy pressure is identified as brittle (or ductile). The measured values of Poisson's ratio (ν) and Cauchy pressure (C_p) validate the brittle characteristics of these alloys.

Table.III.8 illustrates that the elastic anisotropy factor A diverges from unity, suggesting that the alloys being examined display anisotropic characteristics. The material's stiffness is defined by the Young's modulus Y . A greater value of Young's modulus signifies a more robust material. It is evident that Rb_2TiSi exhibits greater stiffness in comparison to Rb_2TiZ (where $Z = Ge, Sn, \text{ and } Sb$) alloys.

Table.III.8 The calculated elastic properties of Rb_2TiZ ($Z = Si, Ge, Sn \text{ and } Sb$) compounds.

Elastic Properties	Rb_2TiSi	Rb_2TiGe	Rb_2TiSn	Rb_2TiSb
$C_{11}(\text{GPa})$	40.704	35.684	35.718	30.541
$C_{12}(\text{GPa})$	10.942	9.937	10.976	14.322
$C_{44}(\text{GPa})$	18.243	16.150	17.014	19.149
Bulk modulus B (GPa)	20.862	18.519	19.223	19.728
Shear modulus G (GPa)	16.897	14.839	15.156	14.732
Poisson's ratio	0.181	0.183	0.187	0.201
Young's modulus Y (GPa)	39.914	35.133	36.005	35.387
Cauchy pressure C_p	-7.301	-6.213	-6.037	-4.827
Pugh ratio, B/G	1.234	1.248	1.268	1.339
Elastic anisotropy factor, A	1.225	1.254	1.375	2.36

To evaluate the dynamic stability of the materials under investigation, we computed the phonon dispersion curves. The primitive cell of Rb_2TiZ (where $Z = \text{Si, Ge, Sn, and Sb}$) consists of 4 atoms, leading to a phonon spectrum characterized by twelve vibrational modes. Among these modes, three are acoustic (two transverse acoustic (TA) and one longitudinal acoustic (LA) branch) and are found at lower frequencies, while nine are optical (three longitudinal optical (LO) and six transverse optical (TO) branches) and are located at higher frequencies. The phonon distribution curves for Rb_2TiSi , Rb_2TiGe , Rb_2TiSn , and Rb_2TiSb are illustrated in [Figure.III.13](#). Given that all phonon branches exist within the positive frequency range, we deduce that these compounds exhibit dynamic stability.

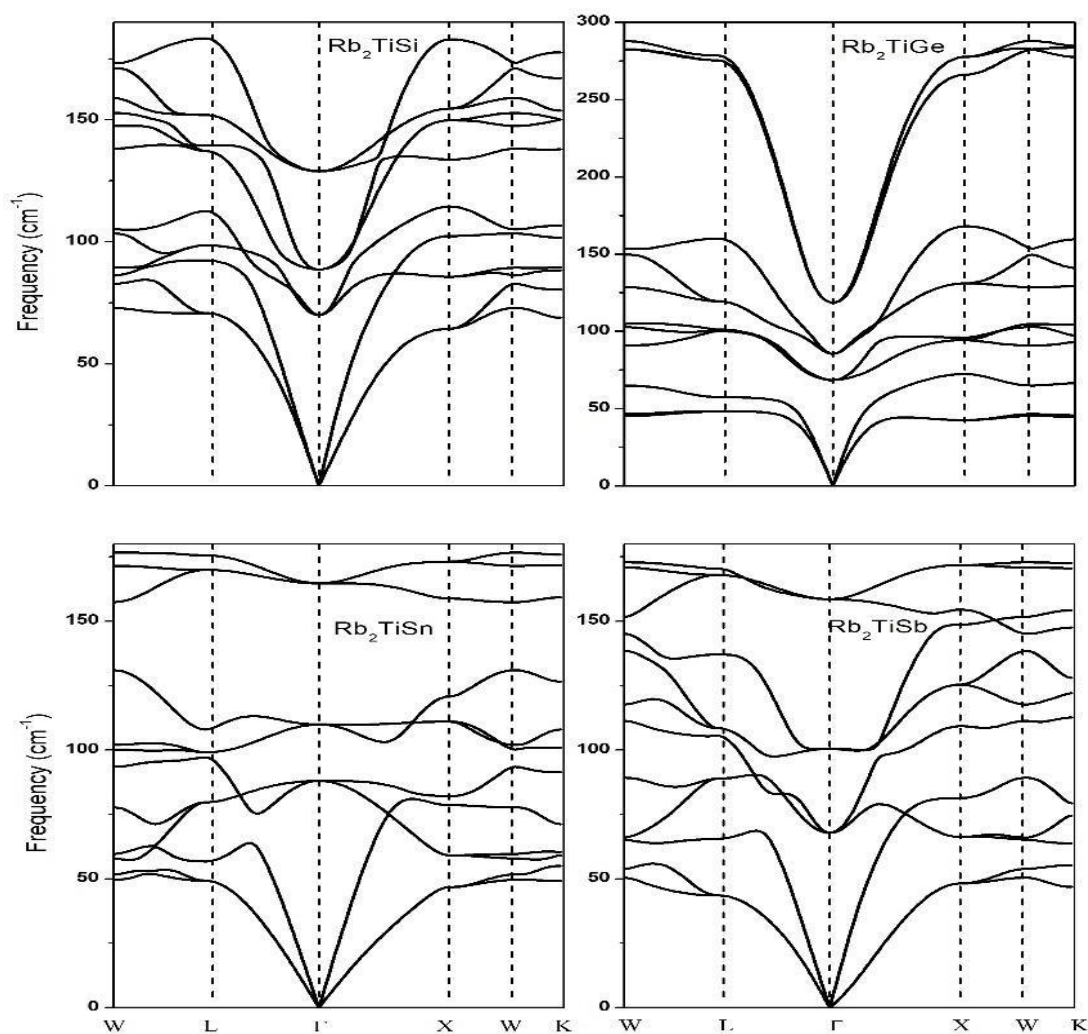


Fig.III.13 calculated phonon dispersion curves for Rb_2TiZ ($Z = \text{Si, Ge, Sn and Sb}$) compounds.

Based on the obtained results from the formation energy, elastic constant, and phonon vibrations, we conclude that Rb_2TiZ ($Z = \text{Si, Ge, Sn and Sb}$) compounds are stable in the FM Hg_2CuTi ground state.

III.4.2 Electronic and magnetic properties

As shown in [Figure.III.14](#), the spin-polarized band structures at the equilibrium lattice constant were computed using the GGA and GGA+mBJ methods. The band structures derived from GGA calculations reveal that the conduction band minimum (CBM) and valence band maximum (VBM) of Rb_2TiSb are located in the spin-down channel at -0.197 eV and -1.440 eV, while in the spin-up channel, they are found at 0.225 eV and 0.010 eV, respectively.

The semiconductor character is lost since the Fermi level intersects with one of the two bands in the two-spin direction. Consequently, a pseudo-gap of 0.215 and 1.243 eV is formed in the spin-up and spin-down channels, respectively. In the case of Rb_2TiGe , we observed that the majority spin exhibits metallic properties while the minority spin behaves as a semiconductor, featuring an indirect band gap ($X-\Gamma$) of approximately 0.482 eV. This observation indicates that the Rb_2TiGe Heusler compound possesses a half-metallic nature in its equilibrium state.

The appearance of an energy band gap in both the spin-up and spin-down channels within the band structures of Rb_2TiSi and Rb_2TiSn signifies the presence of semiconducting states in both spin orientations. The band structures for Rb_2TiSi and Rb_2TiSn reveal an indirect ($W-X$) band gap of 0.135 eV and 0.077 eV in the spin-up direction, along with a direct band gap of 0.836 eV and 0.801 eV at the X point in the spin-down channel, respectively.

The spin-polarized band structures of Rb_2TiZ ($Z = \text{Si, Ge, Sn, and Sb}$) compounds using mBJ potential are presented in [Figure.III.14](#). A notable shift in the electronic properties has been observed. All Rb_2TiZ ($Z = \text{Si, Ge, Sn, and Sb}$) compounds exhibit semiconductor characteristics in both spin directions, highlighting their magnetic semiconducting nature.

This figure indicates that the band structures of Rb₂TiSb differ significantly from those of Rb₂TiZ (Z = Si, Ge, and Sn) alloys. When the mBJ approximation is applied, the valence band maximum (VBM) for Rb₂TiSb shifts downward, while the conduction band minimum (CBM) shifts upward in the minority spin channel. Conversely, for Rb₂TiZ (Z = Si, Ge, and Sn) compounds, both the VBM and CBM are elevated to higher energy levels. Additionally, the conduction band minimum increases for all compounds in the majority spin channel.

Table.III.9 reflects the results derived from the band structures using the GGA and mBJ approximations. Under the mBJ scheme, the band gap has further increased in both spin channels. It is acknowledged that GGA tends to underestimate the energy band gaps of semiconductors and insulators [58-61]. In the majority spin states, the band gap attains values of 1.133 eV, 0.922 eV, 1.068 eV, and 0.024 eV, while in the minority spin states, it reaches 1.248 eV, 1.022 eV, 1.180, and 2.184 eV, for Rb₂TiSi, Rb₂TiGe, Rb₂TiSn, and Rb₂TiSb, respectively.

Table.III.9 the computed formation E_f (eV), cohesive E_c (eV) and band gap energies E_g (eV) of Rb₂TiZ (Z = Si, Ge, Sn, and Sb) compounds.

Compounds	E_f	E_{coh}	E_g			
			GGA		mBJ	
			up	dn	up	dn
Rb ₂ TiSi	-2.83	-8.39	0.135	0.836	1.133	1.248
Rb ₂ TiGe	-2.48	-7.99	-	0.482	0.922	1.022
Rb ₂ TiSn	-2.13	-7.86	0.077	0.801	1.068	1.180
Rb ₂ TiSb	-1.43	-8.19	-	-	0.024	2.184

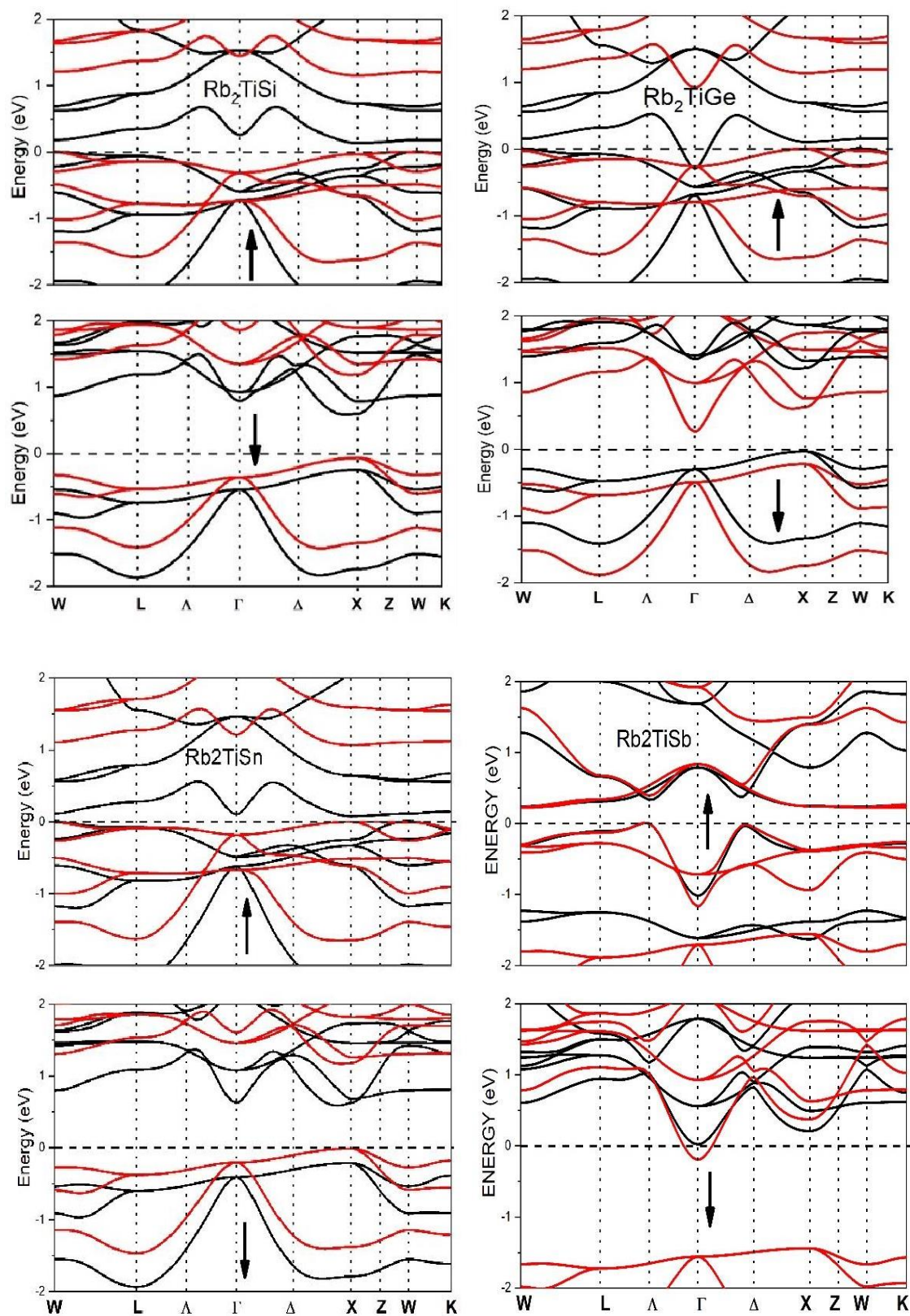


Fig.III.14. Band structures of Rb_2TiZ ($Z = \text{Si, Ge, Sn}$ and Sb) alloys calculated within GGA (black lines) and GGA+mBJ (red lines) approaches.

To account for relativistic effects in these compounds, we conducted electronic-structure calculations that explicitly incorporate spin–orbit coupling (SOC). The inclusion of SOC enables a rigorous assessment of the stability of our initial conclusion regarding the magnetic semiconducting character of the Rb_2TiZ alloys. Since SOC introduces mixing between spin-up and spin-down electronic states, the spin character and bandgap were analyzed using the fat-band formalism together with the spin-resolved density of states (DOS). The resulting SOC-influenced band structures of the Rb_2TiZ systems are displayed in [Fig.III.15](#).

The obtained band-gap values for all compounds are presented in [Table.III.10](#). The fundamental electronic character of these materials remains unaltered by the inclusion of spin–orbit coupling (SOC), irrespective of whether the GGA or mBJ approximation is employed. Significantly, the incorporation of SOC within the mBJ scheme does not compromise the magnetic semiconducting behavior initially predicted; rather, it fully confirms this characterization. Consistent with known limitations of the GGA functional, the mBJ and mBJ + SOC calculations yield substantially larger band gaps for all compounds compared with the GGA and GGA + SOC results. Furthermore, the mBJ + SOC dataset reinforces the conclusions drawn from the mBJ calculations, without introducing any qualitative deviations. Another noteworthy observation is that the addition of SOC to the GGA functional does not modify the overall electronic trends inherent to GGA. Depending on the compound and spin channel, SOC induces only minor adjustments to the band-gap values, producing slight increases or decreases.

The influence of spin–orbit coupling (SOC) in Heusler alloys is strongly dependent on the specific compound and the physical properties being examined. A widely recognized conclusion, originating from the work of Mavropoulos et al. [\[62-64\]](#), indicates that SOC exerts only a minimal impact on spin polarization and half-metallicity in many Heusler systems, typically reducing the polarization by merely 1–2%. This small effect has frequently justified neglecting SOC in studies focused primarily on these properties [\[65-70\]](#). Nevertheless, this overall trend

admits notable exceptions, particularly in cases where the properties of interest exhibit a pronounced sensitivity to relativistic interactions [71-73].

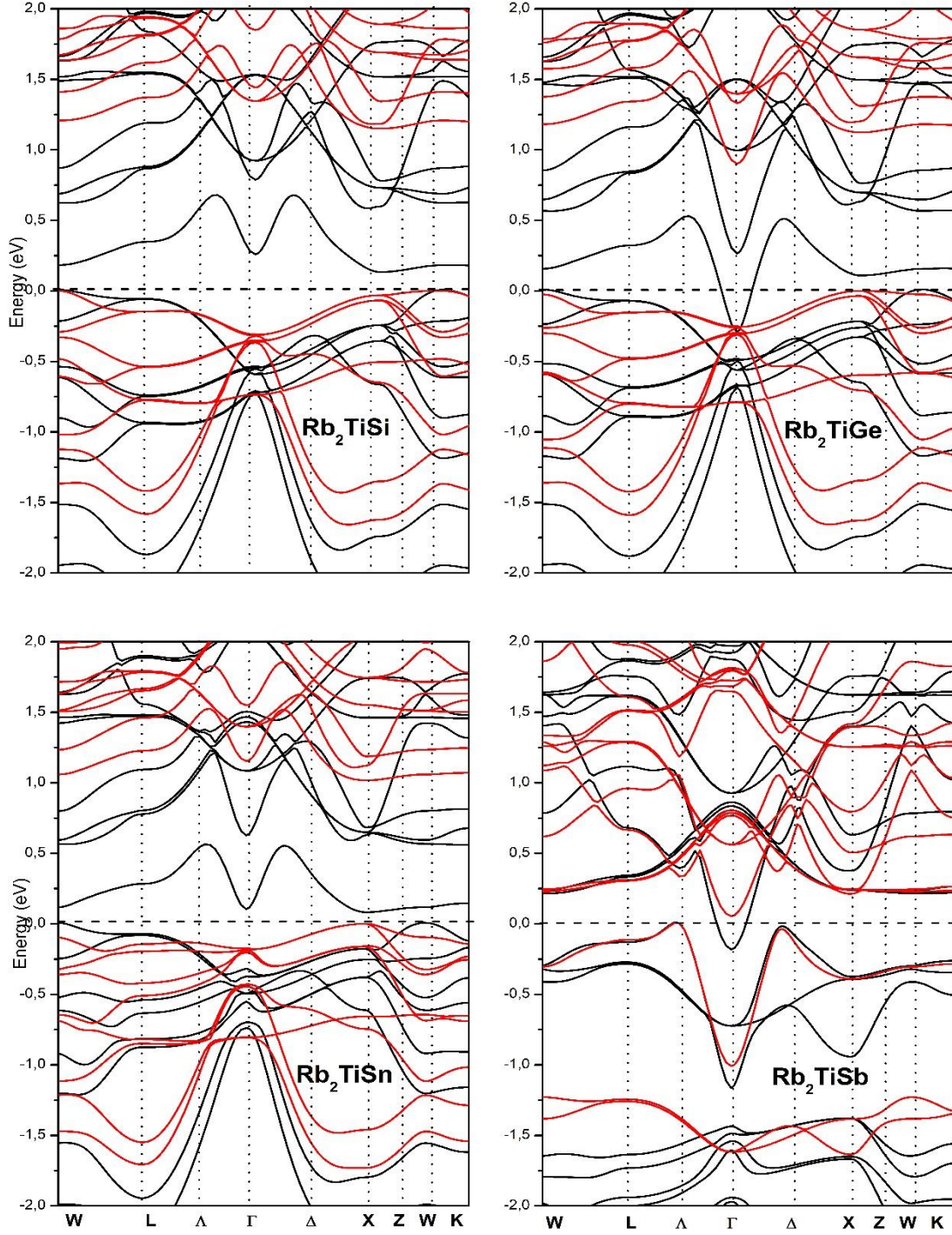


Fig.III. 15. The resulting SOC-influenced Band structures of Rb₂TiZ (Z = Si, Ge, Sn and Sb) systems calculated within GGA (black lines) and GGA+mBJ (red lines) approaches.

Table.III.10. The computed band gap energies E_g (eV) of Rb_2TiZ ($Z = Si, Ge, Sn, \text{ and } Sb$) compounds using GGA and GGA +SOC and mBJ and mBJ + SOC.

Compounds	E_g							
	GGA		GGA+SOC		mBJ		mBJ+SOC	
	up	dn	up	dn	up	dn	up	dn
Rb_2TiSi	0.135	0.836	0.134	0.828	1.133	1.248	1.15	1.250
Rb_2TiGe	-	0.482	-	0.519	0.922	1.022	0.902	1.023
Rb_2TiSn	0.077	0.801	0.082	0.813	1.068	1.18	1.01742	1.266
Rb_2TiSb	-	-	-	-	0.24	2.184	0.237	2.094

Figure.III.16 illustrates the total and partial density of states of the Rb_2TiZ ($Z = Si, Ge, Sn, \text{ and } Sb$) compounds compound at optimized geometry.

According to GGA calculations, there are only a limited number of states present at the Fermi energy in the majority-spin states of Rb_2TiGe , as well as for both the majority and minority spin states of Rb_2TiSb , which renders the corresponding spins metallic.

Thus, when treated with mBJ approximation, both the majority and minority spin-occupied and unoccupied states of Rb_2TiZ ($Z = Si, Ge, \text{ and } Sn$) exhibit an upward shift in their total density of states (TDOS). For Rb_2TiSb , the occupied and unoccupied states of the majority experience a downward shift. Conversely, the occupied states of the minority spin shift to lower energies, and the unoccupied states shift to higher energies, aligning with the characteristics of the spin-polarized band structures.

For Rb_2TiZ ($Z = Si, Ge, \text{ and } Sn$), the Fermi level is located closer to the valence band than the conduction band in both spin directions, indicating a p-type behavior [74] In contrast, the spin down state of Rb_2TiSb exhibits n-type behavior since the Fermi level lies just below the conduction band minimum.

It is important to highlight that close to the Fermi level, both GGA and mBJ calculations indicate that the Ti element is predominant in the conduction and valence states within the spin-up channel. In the spin-down channel, Ti continues to dominate the conduction states,

whereas Sb takes precedence in the valence states. Rb atoms show minimal contributions in both the valence and conduction states near the Fermi level.

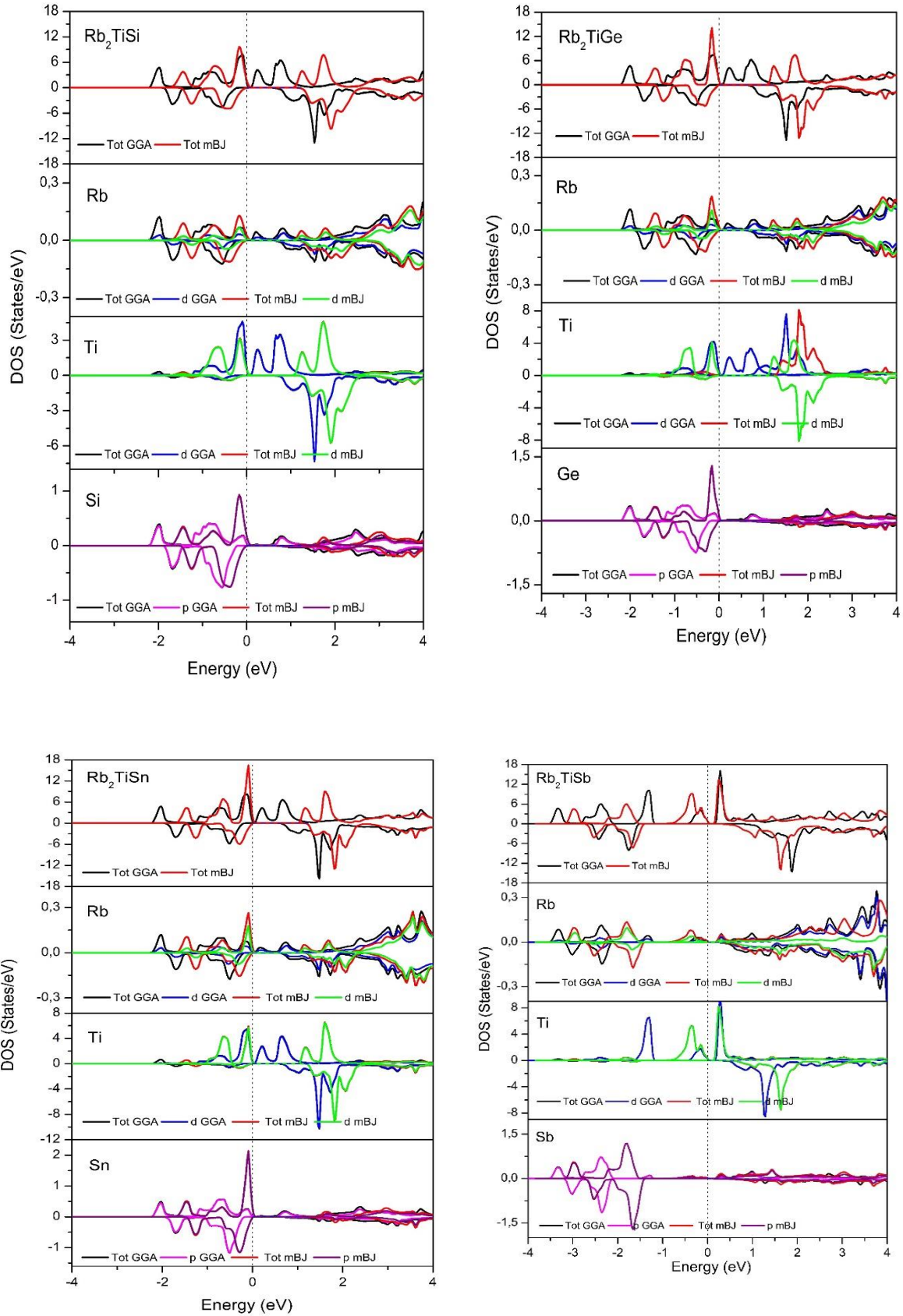
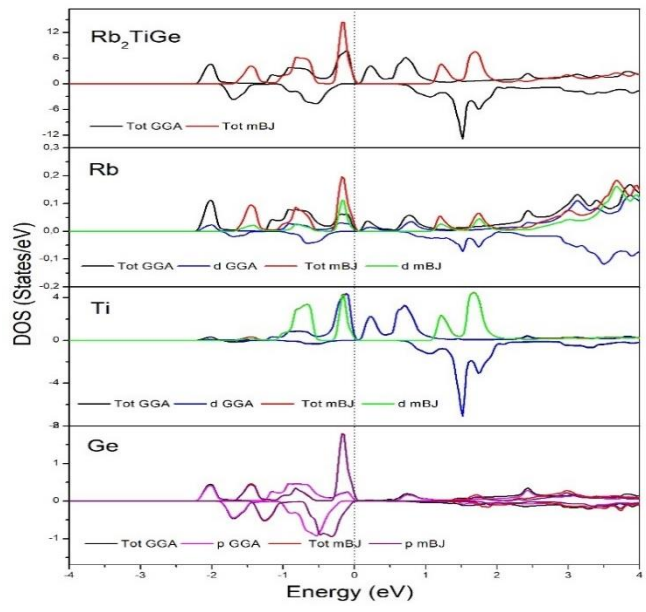
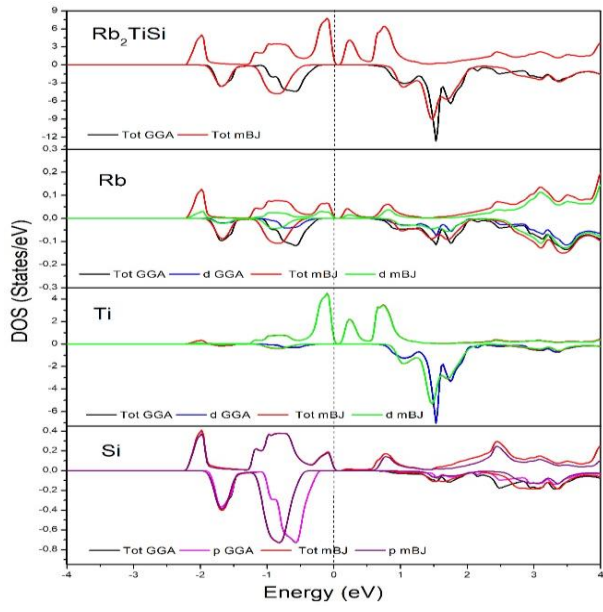


Fig.III.16. Total densities of states (TDOS) and partial densities of states total (PDOS) of Rb_2TiZ ($Z = \text{Si, Ge, Sn and Sb}$) alloys calculated within GGA and GGA+mBJ approaches.

[Fig.III.17](#) presents the total and partial density-of-states (DOS) plots of Rb_2TiZ obtained with SOC included, it is evident that both the T-DOS and PDOS profiles remain essentially unchanged. The influence of SOC on the electronic structure of Rb_2TiZ is therefore extremely small. Consequently, the magnetic semiconducting behavior identified for Rb_2TiZ ($Z = \text{Si, Ge, Sn}$) can be regarded as a robust result, upheld even when relativistic spin-orbit interactions are incorporated. For both the GGA (GGA + SOC) and mBJ (mBJ + SOC) calculations, the TDOS of Rb_2TiZ ($Z = \text{Si, Ge, Sn, and Sb}$) exhibits pronounced features in both the majority- and minority-spin channels, with the dominant contributions arising from Ti-d, Rb-d, and Z-p states. This commonly indicates the d-d and p-d hybridization [\[75, 76\]](#) leading to the conclusion that the p-states of Z elements contribute to gap formation.

Consistent findings have been reported in prior studies [\[77-80\]](#), which likewise demonstrate that the p orbitals of the Z atom strongly hybridize with the d orbitals of the transition-metal atoms. This p-d hybridization is the key factor governing the placement of the Fermi level as well as the magnitude of the minority-spin band gap.

Furthermore, the observation that neither the band-gap values nor the DOS characteristics exhibit any appreciable dependence on SOC provides additional confirmation that the electronic structure is primarily dictated by this robust p-d hybridization, with SOC acting only as a secondary perturbative influence.



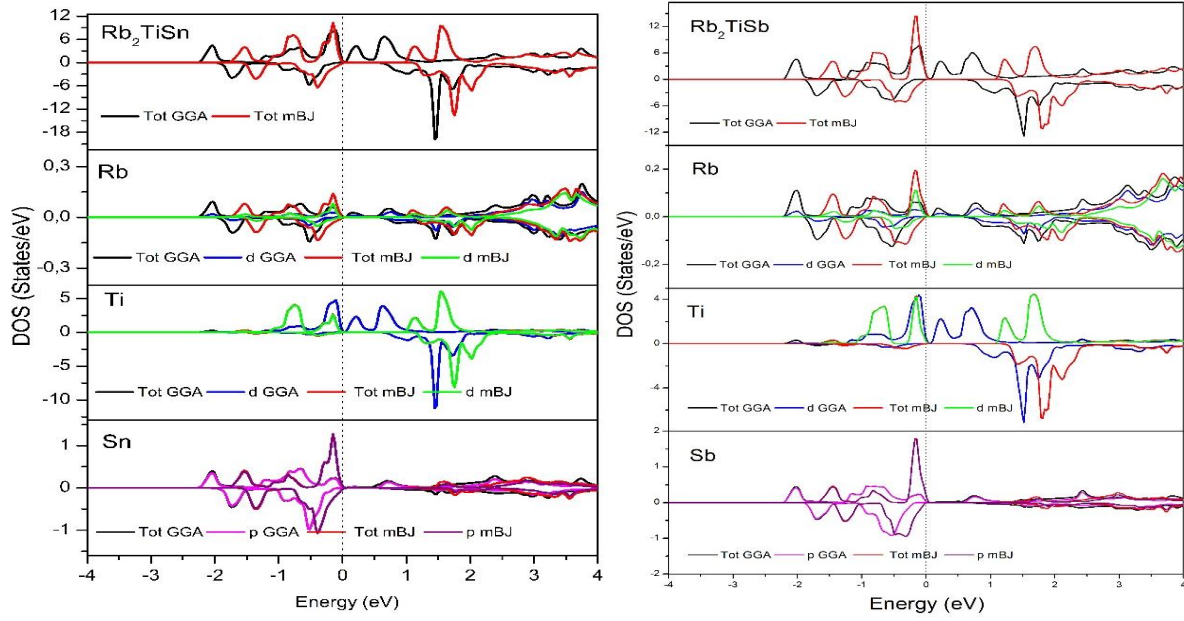


Fig.III.17. The resulting SOC-influenced total densities of states (TDOS) and partial densities of states total (PDOS) of Rb_2TiZ ($Z = \text{Si, Ge, Sn and Sb}$) alloys calculated within GGA and GGA+mBJ approaches.

[Table.III.11](#) lists the total and partial magnetic moments of Rb_2TiZ ($Z = \text{Si, Ge, Sn and Sb}$) as determined by the GGA and mBJ techniques. For Rb_2TiZ ($Z = \text{Si, Ge, and Sn}$), the magnetic moment per formula unit is $2.00 \mu_B$, whereas for Rb_2TiSb , it is $3.00 \mu_B$.

The calculated total magnetic moment M_t of a these full-Heusler alloys follows the general Slater-Pauling rule [81,83] given by $M_t = (Z_t - 8) \mu_B$. Here, Z_t is the total number of valence electrons, which is equal to 10 for Rb_2TiZ ($Z = \text{Si, Ge, and Sn}$) and 11 for Rb_2TiSb .

The total magnetic moment is primarily attributable to the Ti atom and the interstitial zone, with minimal contributions from the Rb and Z.

Moreover, these compounds exhibit ferrimagnetic semiconductor characteristics due to the anti-parallel alignment of atomic magnetic moments between the Z atom and the other atoms.

The data summarized in [Table.III.11](#) demonstrate that the incorporation of SOC leads to only minimal modifications in both the total and atom-resolved magnetic moments across all studied compositions and computational approaches.

Within the GGA approximation, the total magnetic moments remain effectively invariant

upon inclusion of SOC, with changes not exceeding 0.005 μ_B . The integer values of the total magnetic moments approximately 2 μ_B for Z = Si, Ge, and Sn, and 3 μ_B for Z = Sb are fully preserved, thereby confirming the half-metallic or magnetic semiconducting nature of these alloys. A comparable trend is observed under the mBJ scheme, where the mBJ + SOC calculations yield total magnetic moments nearly indistinguishable from those obtained without SOC. These results collectively indicate that the spin polarization and magnetic ordering in Rb_2TiZ are exceptionally robust with respect to relativistic spin–orbit interactions.

Table. III.11 Total M_{tot} (μ_B) and partial magnetic moments M_{ATOM} (μ_B) of Rb_2TiZ (Z = Si, Ge, Sn and Sb) as determined by the compounds using GGA (GGA +SOC) and mBJ (mBJ + SOC) Approximations.

Compound	Approx	MInterstitial	M_{Rb1}	M_{Rb2}	M_{Ti}	M_Z	M_{tot}
Rb_2TiSi	GGA	0.643	0.008	0.007	1.431	-0.089	2.00
	GGA+SOC	0.643	0.008	0.007	1.43	-0.088	2.00
	mBJ	0.58	0.008	0.007	1.454	-0.049	2.00
	mBJ+SOC	0.58	0.008	0.007	1.448	-0.043	2.00
Rb_2TiGe	GGA	0.622	0.006	0.006	1.44	-0.074	2.00
	GGA+SOC	0.647	0.006	0.006	1.44	-0.099	2.00
	mBJ	0.623	0.006	0.006	1.437	-0.072	2.00
	mBJ+SOC	0.629	0.006	0.006	1.456	-0.097	2.00
Rb_2TiSn	GGA	0.375	0.006	0.006	1.71	-0.097	2.00
	GGA+SOC	0.638	0.003	0.003	1.44	-0.084	2.00
	mBJ	0.34	0.006	0.006	1.69	-0.042	2.00
	mBJ+SOC	0.574	0.004	0.004	1.456	-0.038	2.00
Rb_2TiSb	GGA	1.324	0.019	0.02	1.689	-0.051	3.00
	GGA+SOC	1.36	0.029	0.03	1.681	-0.097	3.00
	mBJ	1.229	0.019	0.02	1.773	-0.041	3.00
	mBJ+SOC	1.268	0.024	0.025	1.771	-0.088	3.00

We will now focus on the study of the exchange splitting energy, ΔE_{ex} [84], and the Curie temperature [85] of the compounds under investigation.

The exchange splitting of the conduction band in a magnetic semiconductor alloy is a fundamental factor for spin filtering, expressed as:

$$\Delta E_{ex} = \frac{1}{2} (E_{spin-up} - E_{spin-down}) \quad (10)$$

Where $E_{spin-up}$ and $E_{spin-down}$ are the energy positions of the minima of the conduction bands for the spin-up and spin-down states, respectively.

The computed exchange splitting energies of the Rb_2TiZ full Heusler alloys, using GGA and mBJ approximations are presented in Table.III.12.

Within GGA approach, the estimated values of $2\Delta E_{ex}$ for Rb_2TiSn and Rb_2TiSi are comparable to the exchange splitting of the most studied ferromagnetic semiconductors for spintronics, such as the Eu chalcogenides and EuX ($X = S$ and Se) [86,90].

For all compounds, the discrepancy between GGA and mBJ calculations of the exchange splitting energy is substantial.

While using mBJ approximation, the exchange splitting energy increased for Rb_2TiSb and Rb_2TiGe , while it decreased significantly for Rb_2TiSn and Rb_2TiSi . The calculated values of $2\Delta E_{ex}$ for Rb_2TiSb and Rb_2TiGe are close to previously reported values of other full and quaternary Heusler spin filter materials [91].

The Curie temperature is an important physical property of solids in the technological applications. Using the mean field approximation, the Curie temperature can be computed with the following formula [92,93]:

$$T_C = \frac{2}{3k_B} (E_{NM} - E_{FM}) \quad (11)$$

Where E_{NM} and E_{FM} are the total energies of the non-magnetic and ferromagnetic phases, respectively and k_B is the Boltzmann constant. The predicted Curie temperatures of our compounds are presented in Table.III.12. Thus, Rb_2TiZ Heusler alloys possess high Curie temperatures, making them suitable for spin-filters devices.

Table.III.12 The exchange splitting energy and the Curie temperature of Rb_2TiZ ($Z = \text{Si, Ge, Sn}$ and Sb) compounds.

Compounds	$2\Delta E_{\text{ex}}$		TC
	GGA	mBJ	
Rb_2TiSi	0.452	0.033	1244
Rb_2TiGe	-	0.288	-
Rb_2TiSn	0.511	0.102	1243
Rb_2TiSb	-	0.217	1836

III.4.3 Hydrostatic Pressure effect

In this section, the effect of hydrostatic pressure on the spin-dependent band-gap evolution of the Rb_2TiZ ($Z = \text{Si, Sb}$) compounds is investigated in order to understand the pressure-induced modifications in their electronic properties.

Fig.III. 18 shows that for Rb_2TiSi , the variation of the spin-resolved band gaps reveals a strong dependence on the applied hydrostatic pressure. At -4 GPa, both spin channels exhibit zero band gap, indicating a metallic behavior. At -2 GPa, the spin-up channel remains gapless while the spin-down channel opens a finite band gap of about 0.51 eV, leading to a half-metallic character. For pressures ranging from 0 to 10 GPa, finite band gaps are observed in both spin channels, confirming that the compound maintains its semiconducting behavior under positive hydrostatic pressure. Moreover, the spin-up band gap gradually increases with pressure, whereas the spin-down band gap reaches a maximum value near 0 GPa and then decreases progressively with further pressure increase.

In contrast, Rb_2TiSb exhibits no band gap in either spin channel throughout the entire investigated pressure range, confirming the persistence of its metallic character under hydrostatic pressure.

Table. III. 13. Calculated lattice constants a_0 (Å), and band gap Energy E_g for both spin directions for Rb_2TiSi .

Pressure	a	Eg up	Eg dn
-4	9.079	/	/
-2	8.135	/	0.509
0	7.797	0.135	0.836
2	7.591	0.170	0.797
4	7.443	0.208	0.756
6	7.328	0.219	0.723
8	7.235	0.232	0.692
10	7.156	0.244	0.624

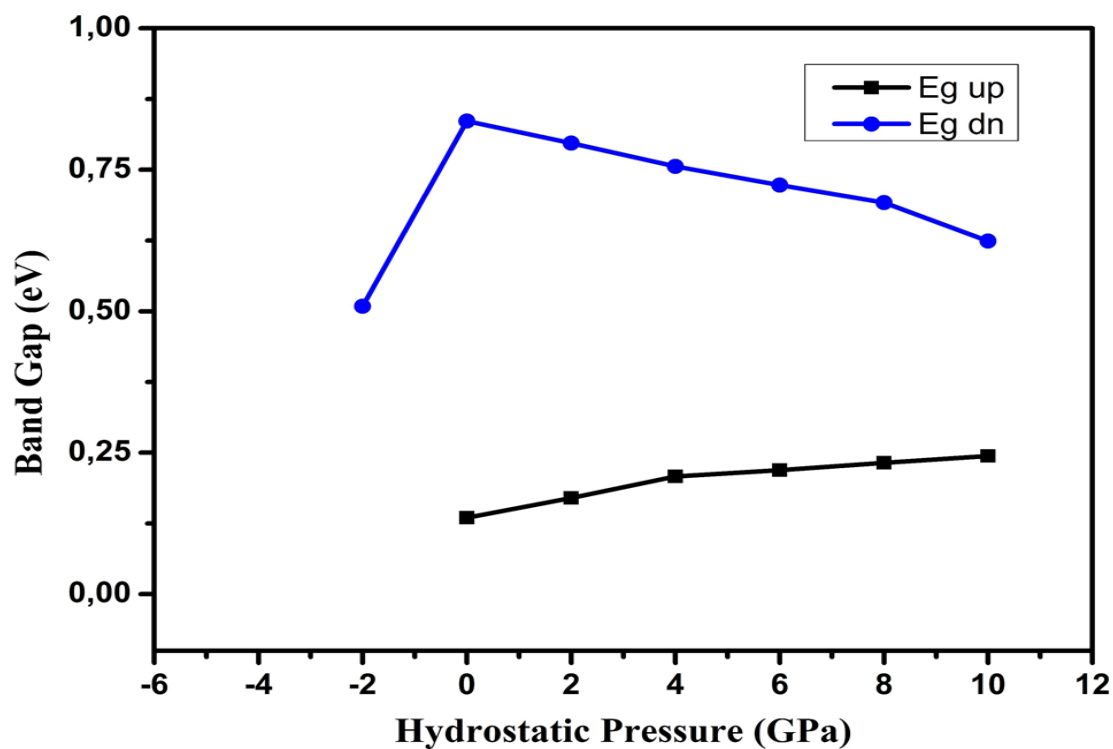


Fig.III.18. Variation of the band gaps in the two spin channels as a function of pressure for Rb_2TiSi .

Table. III. 14. Calculated lattice constants a_0 (Å), and band gap Energy E_g for both spin directions for Rb_2TiSb .

Pressure	a	E_g up	E_g dn
-4	10.521	/	/
-2	8.548	/	/
0	8.14	/	/
2	7.906	/	/
4	7.745	/	/
6	7.618	/	/
8	7.517	/	/
10	7.433	/	/

To conclude, the variation of the total and individual atomic magnetic moments of the Rb_2TiSi and Rb_2TiSb compounds under hydrostatic pressure as illustrated in [Fig.III.20](#) Rb_2TiSi , the total magnetic moment remains nearly constant at approximately 2 μ_B throughout the investigated pressure range, indicating strong magnetic stability under applied pressure. In contrast, the Ti atomic magnetic moment gradually decreases with increasing pressure, while the Si atom preserves a small negative magnetic moment with slight variation. The magnetic moments of the Rb atoms remain very small and nearly unchanged over the entire pressure range.

Similarly, in [Fig.III.21](#) Rb_2TiSb , the total magnetic moment remains almost constant around 3 μ_B , confirming the robustness of the magnetic character under hydrostatic pressure. The Ti atom also exhibits a gradual decrease in its magnetic moment with increasing pressure, whereas the Sb atom maintains a weak negative magnetic moment with minor fluctuations. In addition, the magnetic contributions of the Rb atoms remain negligible throughout the studied pressure interval.

Table. III. 15. Total magnetic moment m_{tot} (μ_B), individual magnetic moments m_X (μ_B) ($X = \text{Rb}, \text{Ti}, \text{Si}$) and interstitial magnetic moment m_{Inter} (μ_B) of Rb_2TiSi Heusler compound under

Hydrostatic pressure.

Pressure	$m_{\text{tot}}(\mu_B)$	$M_{\text{Rb}}(\mu_B)$	$M_{\text{Rb}}(\mu_B)$	$m_{\text{Ti}}(\mu_B)$	$M_Z(\mu_B)$	$m_{\text{Inert}}(\mu_B)$
-4	1.99928	-0.00081	0.00370	1.60036	-0.12964	0.52567
-2	2.00873	0.00412	0.00558	1.47874	-0.09890	0.61920
0	2.00013	0.0084	0.007	1.43121	-0.08701	
2	2.00075	0.01077	0.00826	1.40402	-0.08507	0.66276
4	2.00088	0.01335	0.01064	1.38295	-0.08206	0.67722
6	1.99708	0.01557	0.04415	1.36973	-0.08198	0.68312
8	2.00034	0.01776	0.01161	1.35335	-0.07797	0.69560
10	2.00058	0.01977	0.01257	1.34148	-0.07621	0.70297

Table. III. 16. Total magnetic moment $m_{\text{tot}}(\mu_B)$, individual magnetic moments $m_X(\mu_B)$ ($X = \text{Rb}, \text{Ti}, \text{Sb}$) and interstitial magnetic moment $m_{\text{Inter}}(\mu_B)$ of Rb_2TiSb Heusler compound under Hydrostatic pressure.

Pressure	$m_{\text{tot}}(\mu_B)$	$M_{\text{Rb}}(\mu_B)$	$M_{\text{Rb}}(\mu_B)$	$m_{\text{Ti}}(\mu_B)$	$M_Z(\mu_B)$	$m_{\text{Inert}}(\mu_B)$
-4	2.86805	0.00265	0.00800	1.77882	-0.12117	1.19974
-2	2.98287	0.01400	0.02603	1.70561	-0.10664	1.34386
0	3.00011	0.01902	0.02023	1.68903	-0.05101	
2	3.00067	0.02478	0.03745	1.66929	-0.10569	1.37484
4	3.00054	0.02884	0.04110	1.65801	-0.10384	1.37643
6	3.00043	0.03233	0.04415	1.64752	-0.10226	1.37870
8	2.99040	0.03542	0.04650	1.63654	-0.09924	1.37117
10	2.97739	0.03790	0.04823	1.63015	-0.09950	1.36062

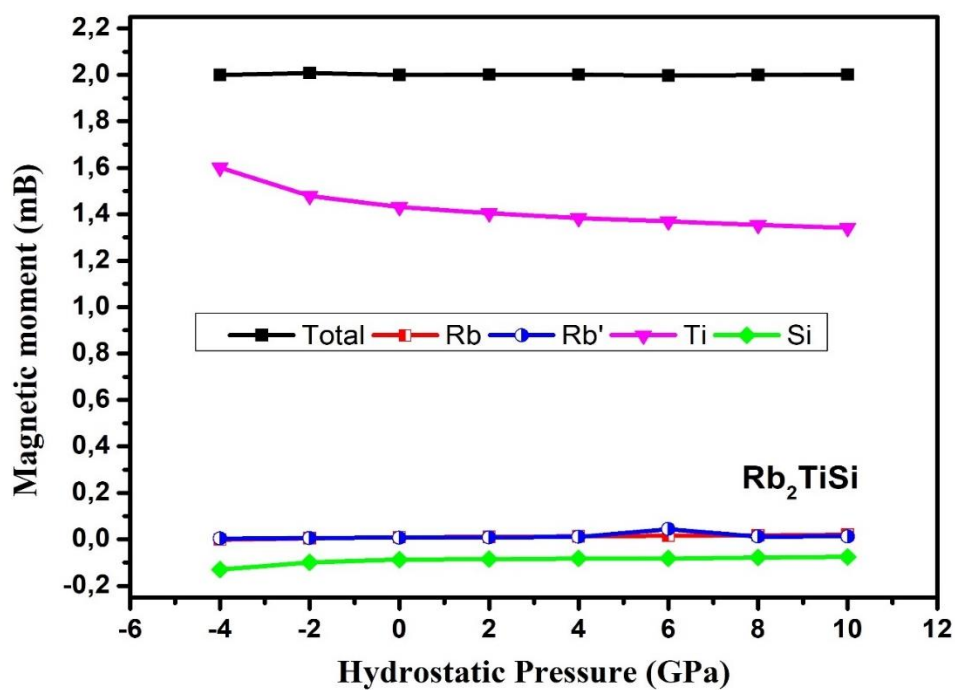


Fig. III.19. Variation of the total and atomic magnetic moments as a function of Hydrostatic pressure for Rb_2TiSi .

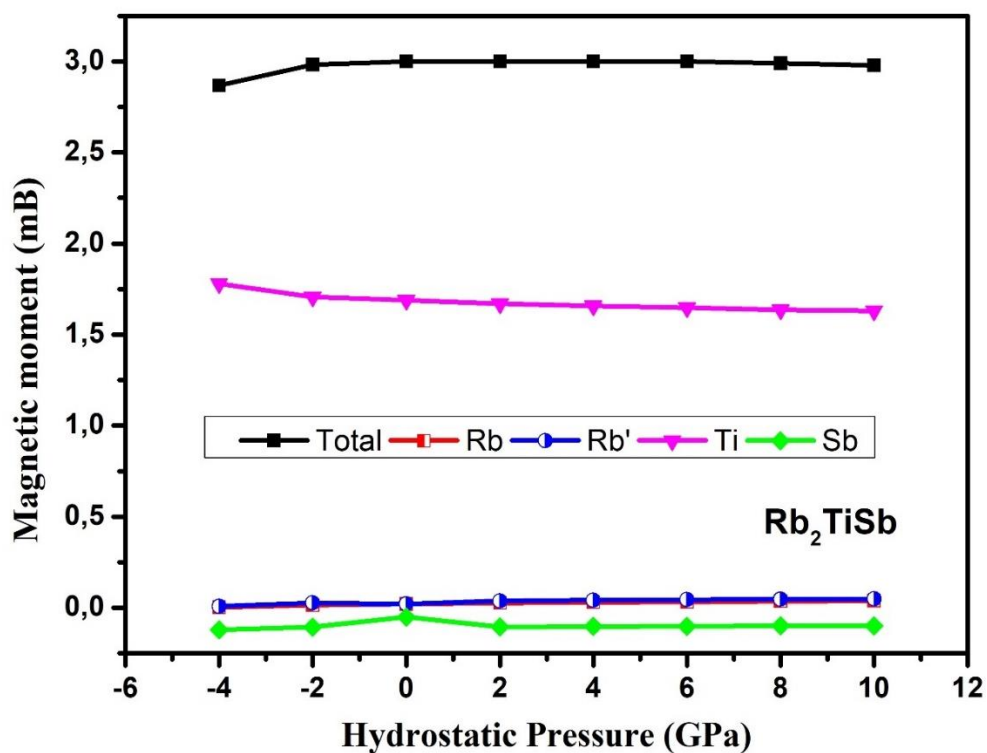


Fig. III.20. Variation of the total and atomic magnetic moments as a function of the Hydrostatic pressure for Rb_2TiSb .

III.4.4 Uniaxial Pressure effect

Uniaxial pressure was applied to investigate the electronic and magnetic properties of the Rb_2TiZ ($Z = \text{Si}, \text{Sb}$) compounds. The spin-resolved band structures were calculated for pressures ranging from 2 to 10 GPa using the GGA approximation.

For Rb_2TiSi , the material preserves its semiconducting nature in both spin channels within the pressure range of 2 to 4 GPa. However, between 6.0 and 10 GPa, the band gap in the spin-down channel takes values of 0.676, 0.622, and 0.568, while the spin-up channel becomes gapless. This transition results in half-metallic behavior.

In contrast, Rb_2TiSb exhibits a gapless electronic structure in both spin channels across the entire pressure range from 2 to 10 GPa, indicating a metallic character.

Table. III. 17. Calculated lattice constants a_0 (Å) and c (Å), and band gap Energy E_g for both spin directions for both Rb_2TiSi .

Rb_2TiSi	a	c	E_g up	E_g dn
0	7.79	7.79	0.135	0.836
2	5.51	7.79	0.101	0.801
4	5.55	7.47	0.068	0.748
6	5.60	7.32	0.0	0.676
8	5.63	7.16	0.0	0.622
10	5.67	7.01	0.0	0.568

Table. III. 18. Calculated lattice constants a_0 (Å) and c (Å), and band gap Energy E_g for both spin directions for Rb_2TiSb .

Rb₂TiSb	a	c	Eg up	Eg dn
0	8.14	8.14	/	/
2	5.79	7.97	/	/
4	5,82	7.81	/	/
6	5,84	7.65	/	/
8	5,90	7.48	/	/
10	5,94	7.32	/	/

Fig.III.21. presents the variation of the band gap in both spin channels as a function of the applied uniaxial pressure for Rb₂TiSi. As pressure increases, the band gap in the spin-down channel decreases steadily and almost linearly over the entire pressure range. In contrast, the spin-up channel shows a rapid reduction in the band gap from 0 to 6 GPa, reaching a zero value at 6 GPa. Beyond this pressure, the band gap remains constant at zero, indicating a gapless state. This behavior suggests a transition toward half-metallicity starting from 6 GPa.

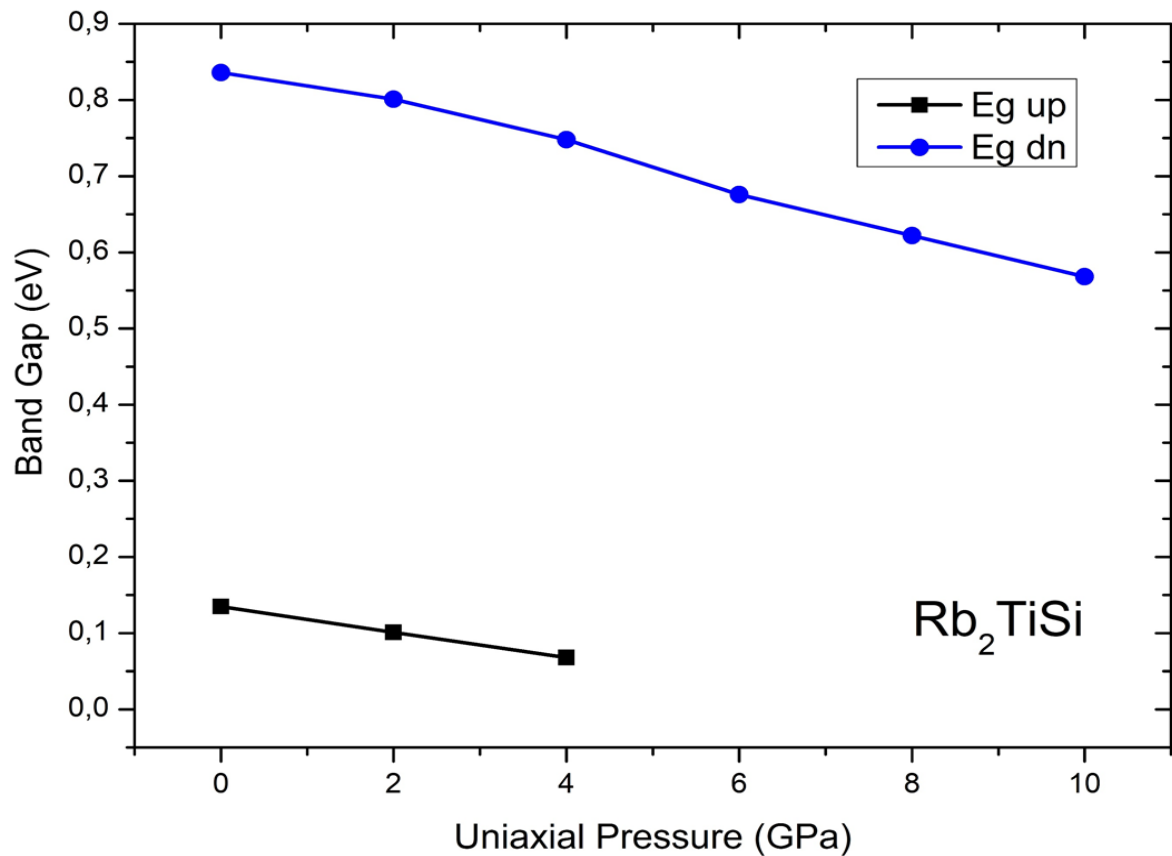


Fig.III.21. Variation of the band gaps in the two spin channels as a function of Uniaxial pressure.

Finally, we investigated the dependence of the total and individual atomic magnetic moments under uniaxial pressure ranging from 0 to 10 GPa for the Rb_2TiSi and Rb_2TiSb compounds. As illustrated in the figures, the total magnetic moment remains nearly constant over the entire pressure range, with values of approximately 2 μB for Rb_2TiSi and 3 μB for Rb_2TiSb , indicating a robust magnetic stability under applied pressure.

For both compounds, the dominant contribution to the total magnetic moment arises from the Ti atom, whose magnetic moment remains almost unchanged with increasing pressure. In contrast, the magnetic moments of the Rb atoms are negligible and show no significant variation. The p-element atoms (Si and Sb) exhibit small negative magnetic moments, which also remain nearly constant across the pressure range. Overall, the invariance of both total and atomic magnetic moments under uniaxial pressure suggests that these compounds preserve their magnetic character and exhibit strong stability against external mechanical perturbations.

Table. III. 19. Total magnetic moment m_{tot} (μB), individual magnetic moments m_X (μB) ($X = \text{Rb}, \text{Ti}, \text{Si}$) and interstitial magnetic moment m_{Inter} (μB) of Rb_2TiSi Heusler compound under uniaxial pressure.

Pressure	$m_{\text{tot}}(\mu\text{B})$	$m_{\text{Rb}}(\mu\text{B})$	$m_{\text{Rb}}(\mu\text{B})$	$m_{\text{Ti}}(\mu\text{B})$	$m_{\text{Si}}(\mu\text{B})$	$m_{\text{Inter}}(\mu\text{B})$
0	2.00013	0.00840	0.00700	1.43121	-0.08701	0.64302
2	2.00087	0.00870	0.00741	1.42339	-0.08749	0.64886
4	2.00037	0.00959	0.00765	1.41683	-0.08699	0.65328
6	1.99962	0.00968	0.00732	1.42408	-0.08914	0.64768
8	2.00151	0.01108	0.00771	1.41962	-0.09018	0.65328
10	2.00166	0.01272	0.00804	1.41512	-0.09164	0.65742

Table. III. 20. Total magnetic moment m_{tot} (μ_B), individual magnetic moments m_X (μ_B) ($X = \text{Rb}$, Ti , Sb) and interstitial magnetic moment m_{Inter} (μ_B) of Rb_2TiSb Heusler compound under uniaxial pressure.

Pressure	$m_{\text{tot}}(\mu_B)$	$M_{\text{Rb}}(\mu_B)$	$M_{\text{Rb}}(\mu_B)$	$M_{\text{Ti}}(\mu_B)$	$M_z(\mu_B)$	$m_{\text{Inert}}(\mu_B)$
0	3.00011	0.01902	0.02023	1.68903	-0.05101	1.32401
2	2.99824	0.02053	0.03315	1.68405	-0.05112	1.31164
4	2.99766	0.02125	0.03334	1.68289	-0.05121	1.31139
6	2.99738	0.02270	0.03405	1.67966	-0.05113	1.31210
8	2.99559	0.02349	0.03332	1.68115	-0.05114	1.30877
10	2.99073	0.02510	0.03304	1.68062	-0.05082	1.30278

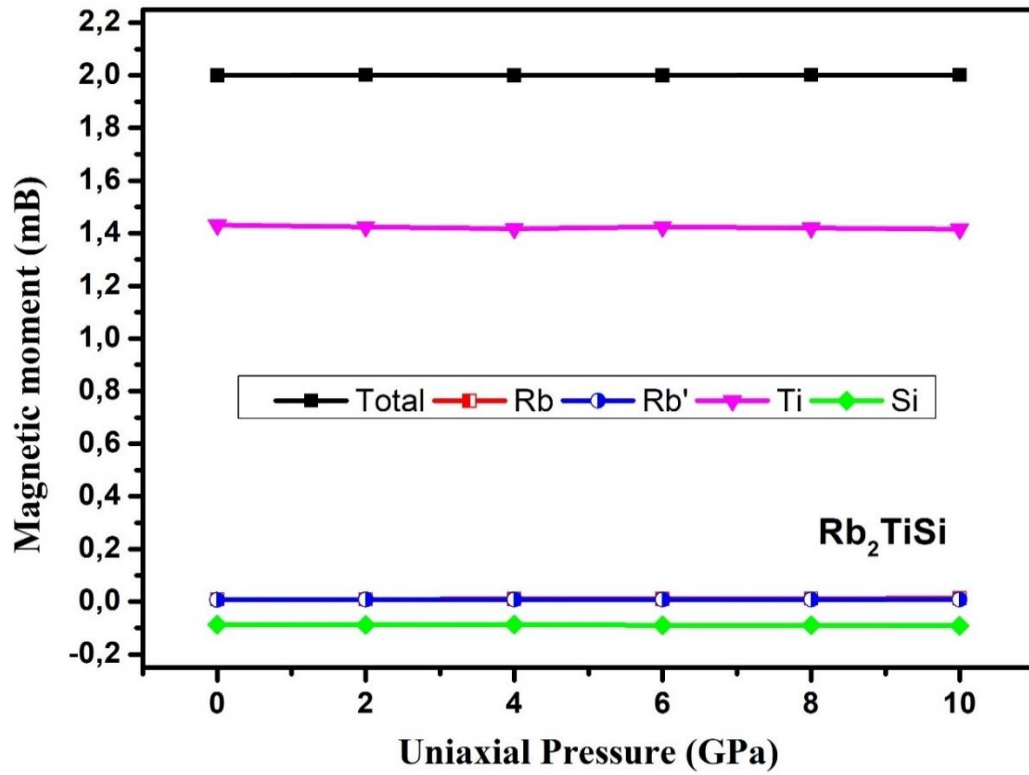


Fig.III.22. Variation of the total and atomic magnetic moments as a function of the uniaxial pressure for Rb_2TiSi .

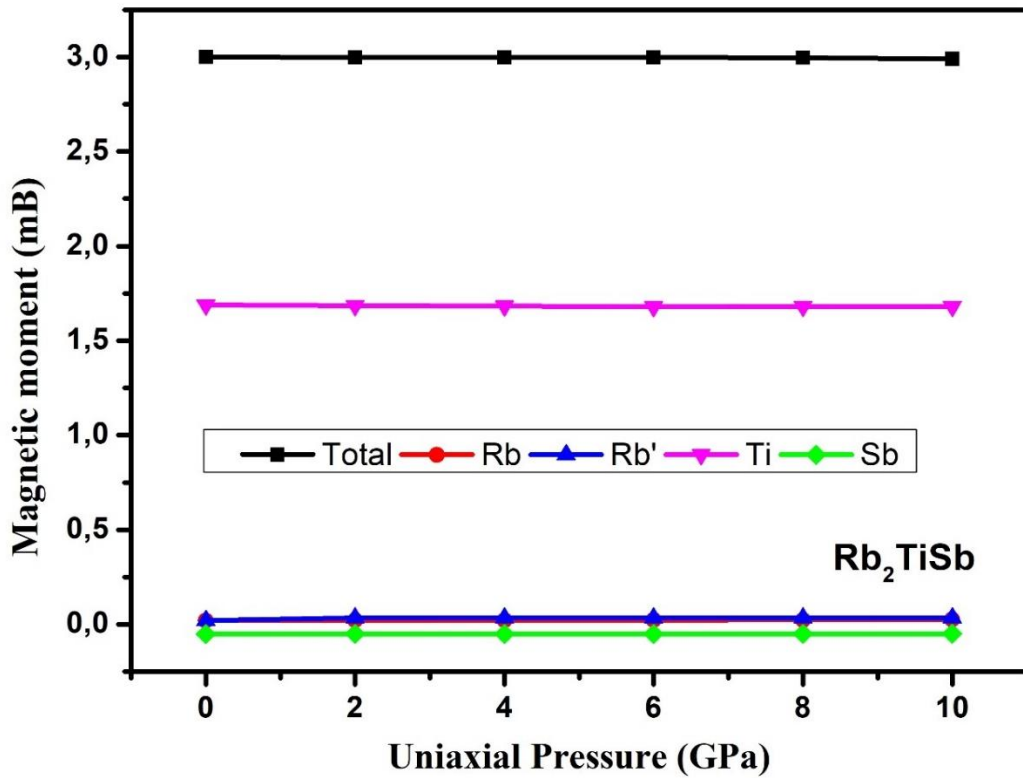


Fig.III.23. Variation of the total and atomic magnetic moments as a function of the uniaxial pressure for Rb₂TiSb.

III.5 Conclusion

Using first-principles calculations, we have examined the structural, electronic, and magnetic properties of the Rb₂TiZ (Z = Si, Ge, Sn, and Sb) compounds. Our results identify the ferromagnetic Hg₂CuTi-type phase as the most energetically favorable configuration. The stability of all proposed alloys is further verified through evaluations of the formation and cohesive energies, elastic constants, and lattice vibrational properties. The Rb₂TiZ systems are predicted to be magnetic semiconductors, with band gaps opening in both spin channels as a direct consequence of strong p–d hybridization. The calculated integer magnetic moments—2.000 μ B for Rb₂TiZ (Z = Si, Ge, Sn) and 3.000 μ B for Rb₂TiSb—are in excellent agreement with the Slater–Pauling relation $M_t = (Z_t - 8) \mu$ B. Overall, the minimal changes observed in both the band-gap values and total magnetic moments upon inclusion of SOC within the GGA and mBJ schemes

indicate that relativistic effects exert only a negligible influence on the electronic and magnetic properties of the Rb_2TiZ compounds

Additionally, the obtained exchange-splitting energies and Curie temperatures are consistent with previously reported experimental and theoretical findings. These results indicate that the Rb_2TiZ compounds are promising candidates for future spin-filter applications. We anticipate that the present work will provide a useful foundation for subsequent experimental and theoretical investigations.

Similarly, the phase stability and magnetism of CoMnTaSb were systematically examined using elastic constants, convex hull analysis, cohesive and formation energies, and phonon dispersions, all of which confirmed its stability and feasibility for experimental synthesis. Both GGA and GGA + mBJ approximations consistently predict its magnetic semiconductor character, with electronic band gaps of 0.196 (0.470) eV in the spin-up and 0.189 (0.441) eV in the spin-down channel, respectively. The total magnetic moment of $2.00 \mu_B$ also satisfies the Slater-Pauling rule and remains constant even under both uniform and non-uniform strain ranging from -10 to 10 GPa, demonstrating robust magnetic semiconductor behavior.

Overall, these findings provide new insights into the design of Heusler alloys with promising spintronic properties. Both the Rb_2TiZ family and CoMnTaSb emerge as strong candidates for future spin-filter applications, encouraging further experimental and theoretical investigations.

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General Conclusion

In this thesis, we applied an ab-initio calculation method based on FP-LAPW with both GGA + mBJ approximations within the framework of Density Functional Theory (DFT), as implemented in the WIEN2k code, to carry out a theoretical investigation of the physical properties under both uniform and non-uniform strain, particularly the structural, electronic, and magnetic properties of both quaternary and full Heusler alloys. The study focused on equilibrium parameters from structural optimization, band structure, total and partial density of states, magnetic moments, and spin polarization for each compound.

The main objective of this work is to identify the properties of a series of materials belonging to Heusler alloys, in which we have selected the novel quaternary compound CoMnTaSb and the full Heusler compounds Rb_2TiZ ($Z = \text{Si, Ge, Sn and Sb}$), in order to determine whether they are good candidates for future spin-filter applications.

In the first part of this work, we focused on the investigation of the novel quaternary compound CoMnTaSb. This choice was primarily motivated by their promising electronic characteristics and the noteworthy values of their magnetic moments. In the second part, we extended our study to a new full Heusler magnetic semiconductor alloy, Rb_2TiZ ($Z = \text{Si, Ge, Sn, and Sb}$), which, to the best of our knowledge, has not been previously examined. The principal results of our investigation are summarized as follows:

- The most important first step is to verify the studied compounds stability: Calculations of the elastic constants, cohesive and formation energies, and phonon dispersion frequencies have demonstrated that the CoMnTaSb compound and Rb_2TiZ ($Z = \text{Si, Ge, Sn, and Sb}$) full Heusler alloys are stable and acceptable for experimental synthesis.
- determine the structural properties of a given system in its ground state: the CoMnTaSb compound tends to crystallize in the Type I structure in the

ferromagnetic (FM) state while The FM-Hg₂CuTi phase is found to be the most stable configuration for the Rb₂TiZ (Z = Si, Ge, Sn, and Sb) compounds.

- Based on the electronic band structure and the total (T-DOS) and partial (P-DOS) density of states calculations within GGA + mBJ approximation, we found that the studied compounds exhibit a magnetic semiconductor character.
- The obtained integer magnetic moment values of 2.000 μ_B for CoMnTaSb and Rb₂TiZ (Z = Si, Ge, and Sn) and 3.000 μ_B for Rb₂TiSb which adheres to the Slater-Pauling rule.
- Under uniform strain ranging from -10 to 10 GPa, the magnetic semiconductor behavior of the CoMnTaSb quaternary Heusler compound is preserved, and the total magnetic moment remains unaffected.
- Under non-uniform strain, the compound preserves its magnetic semiconductor character within the pressure range of 2–6 GPa. At 8 GPa, it undergoes a transition to a half-metallic state, and at 10 GPa it exhibits a metallic behavior.

This study may provide a valuable basis for pursuing more detailed and advanced investigations on complex systems. In this perspective, it would be important to extend the research toward experimental validation in order to confront the theoretical predictions with practical results, as well as to explore additional characteristics such as thermoelectric properties through the use of alternative computational tools.

Abstract

Heusler alloys, a notable class of intermetallic compounds, have attracted considerable interest within materials science and condensed matter physics due to their exceptional combination of mechanical, magnetic, and electronic properties. These characteristics make them highly suitable for diverse applications, including magneto-electronic devices, spintronic technologies, and thermoelectric systems.

This study investigates the effects of hydrostatic and uniaxial pressure on Heusler alloys, with the objective of understanding how external strain influences their electronic band structure, magnetic moments, and optical behavior. The analysis is conducted using Density Functional Theory (DFT) simulations, providing insight into pressure-induced modifications at the atomic and electronic levels. This research contributes to the design and optimization of pressure-tunable spintronic materials, identifying promising Heusler compounds for future magnetic semiconductor and spin-filter device applications.

Key words: FP-LAPW, magnetic semiconductors, Heusler alloys, DFT, spin filter.

Résumé

Les alliages de Heusler, une catégorie remarquable de composés intermétalliques, ont suscité un intérêt considérable dans le domaine de la science des matériaux et de la physique de la matière condensée en raison de leur combinaison exceptionnelle de propriétés mécaniques, magnétiques et électroniques. Ces caractéristiques les rendent particulièrement adaptés à diverses applications, notamment les dispositifs magnéto-électroniques, les technologies spintroniques et les systèmes thermoélectriques.

Cette étude examine les effets de la pression hydrostatique et uniaxiale sur les alliages de Heusler, dans le but de comprendre comment la contrainte externe influence leur structure de bande électronique, leurs moments magnétiques et leur comportement optique.

L'analyse est réalisée à l'aide de simulations basées sur la théorie de la fonctionnelle de la densité (DFT), fournissant un aperçu des modifications induites par la pression aux niveaux atomique et électronique. Cette recherche contribue à la conception et à l'optimisation de matériaux spintroniques ajustables par la pression, en identifiant des composés de Heusler prometteurs pour de futures applications en tant que semi-conducteurs magnétiques et dispositifs filtres de spin.

Mots-clés : FP-LAPW, semi-conducteurs magnétiques, alliages Heusler, DFT, filtre de spin.

المخلص

لقد حظيت سبائك هيوسلر (Heusler) ، وهي فئة مميزة من المركبات البينية المعدنية، باهتمام كبير في مجال علم المواد وفيزياء المادة المكثفة نظراً لتوليفها الفريد من الخصائص الميكانيكية والمغناطيسية والإلكترونية. تجعل هذه الخصائص هذه المواد مناسبة تماماً لمجموعة واسعة من التطبيقات، بما في ذلك الأجهزة المغناطيسية-الإلكترونية وتقنيات الإلكترونيات الدورانية (Spintronics) والأنظمة الحرارية-الكهربائية. تتناول هذه الدراسة تأثير كل من الضغط الهيدروستاتيكي وأحادي المحور على سبائك هيوسلر، بهدف فهم كيفية تأثير الإجهاد الخارجي على البنية الإلكترونية للحزم والعزوم المغناطيسية والخصائص البصرية لهذه المواد. وقد أجريت التحليلات باستخدام حسابات نظرية الكثافة الوظيفية (DFT) ، مما أتاح فهماً أعمق للتغيرات البنيوية والإلكترونية الناتجة عن تطبيق الضغط. تساهم هذه الأبحاث في تصميم وتحسين المواد الدورانية القابلة للضغط بالضغط، مع تحديد سبائك هيوسلر الواعدة لاستخدامها في أشباه الموصلات المغناطيسية ومرشحات الإلكترونات الدورانية (Spin-Filter) المستقبلية.

الكلمات المفتاحية : FP-LAPW , أشباه الموصلات المغناطيسية، سبائك هيوسلر، DFT، مرشح الإلكترونات الدورانية.