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THEME

AB-INITIO CALCULATION OF THE PHYSICAL PROPERTIES OF $XFeB_4$ (X = Y and Sc).

Publicly supported before the jury composed by:

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Thanks

I complete my happiness as I put the last touches of the research, to thank God Almighty for his success in completing this humble work, and to thank those who deserve it, for without them this research would not be completed.

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To classmates, of Physics Applied 2019 /2020 and I ask God for success for all that He loves and which pleases Him

DEDICATION

To my beloved family

To the Honorable Professor Ahmed Gueddouh

To beloved Palestine and free Jerusalem, its eternal capital. To the martyrs of the Arab world and the prisoners behind bars

To my girlfriends, all in her name

To the physics students batch

To students of science and knowledge enthusiasts everywhere. ... and to those who supported this research.

We dedicate this humbel work

TABLE OF CONTENT

Liste Of Obbreviation

GPa	Giga Pascal
DFT	Density Functional Theory
GGA	Generalized Gradient Approximation
TM	Transition Metal
PP-LAPW	Pseudo Potential Linearized Augmented Plane Wave
CASTEP	Cambridge Serial Total Energy Package
PBE	Perdew-Burke Ernzerhof
Cij	Elastic Constants
Sc, Fe, B, Y	Scandium, Iron, Boron, Yttrium
LSDA	Local Spin Density Approximation
$\hat{H}$	the Hamiltonian
$\hat{T}_N$	kinetic energy of nuclei
$\hat{T}e$	kinetic energy of electrons
BOA	Born-Oppenheimer Approximation
Ψ	wave function
$V_{ext}(\mathbf{r})$	Static external potential
HK	Hohenberg-Kohn
$\rho(\mathbf{r})$	Charge density
KS	Kohn and Sham
BZ	Brellouin Zone
LDA	Local Density Approximations.
T_C	*Curie* temperature
FM	Ferromagnetic
B	Bulk modulus of a material
Hv	Hardness
MPA	Mulliken Population Analysis
LCAO	Linear Combined Atomic Orbitals
$\tilde{C}_{ij}$	Elastic Constants under pressure
VRH	Voigt-Reuss-Hill
G	Shear modulus
E	Young modulus
ν	Poisson ratio

A_U	Universal anisotropic factor
S_{ij}	Compliance Matrix
l_1, l_2 and l_3	The direction cosines
Θ_D	Debye temperature
3D	Three dimensional
E_{coh}	Cohesive energy
E_f	Formation energy
E_{total}	Total cell energy
DOS	Density of state
USP	Ultra soft pseudo potentiel
SG	Space groupe
USV	Ultra Soft Vanderbilt

1 General introduction

Materials are crucial in the development of civilization and the improvement of human life. As an example of these materials, Rare earth elements (REEs) with their exceptional magnetic and conductive properties, they enable the hardware of contemporary life to be faster, lighter, and stronger (One method in processing gold ore, simply put, is to mix the ore with sodium cyanide (NaCN). The gold is then leached right out).

Rare earth elements (REEs) are not particularly "rare" in terms of abundance, but for many years remained rarely separated from each other owing to their similar chemical characteristics .Although REEs are widely distributed geographically, they are chiefly mined, concentrated, and separated in China.

First step aims of this work, is to conduct a literature research about rare earth materials metalloids and transitions metals , and in the second step choose some combined materials (rare earth element, metal transition and metalloid element) as a super-hard materials for their a crucial importance and their wide applications, from wear resistant coatings, high hardness to cutting and polishing tools.

For a fundamental understanding of the electronic structure and therefore of the properties of materials, the so-called ab initio method, based on fundamental quantum theory, uses only atomic constants as input parameters for the resolution of the Schrödinger equation. This method has now become a basic tool for studying structural, electronic, mechanical, optical, etc. properties. It is also a tool of choice for the study of certain effects that are difficult or impossible to determine by experimental means and for the prediction of new materials, and it can sometimes replace very expensive or even impractical laboratory experiments. The power of ab-initio calculations comes from the formalism of the density functional theory (DFT) and its two approximations of the energy of exchange and correlation: the local density approximation (LDA) and the generalized gradient approximation (GGA).

In my end of study project, the structural, electronic and mechanic properties of $XFeB_4$ (X = Y and Sc) compounds have been studied using Density Functional Theory (DFT)

This work is divided into three chapters as well as a general introduction and a general conclusion.

chapters I and II are rather theoretical in nature while chapter III is devoted to calculation details and the results obtained during numerical calculations on XFeB4 (X= Y and Sc) compounds.

The first chapter is a bibliographic research on rare earth materials and their uses, metalloids and transition elements.

Chapter II presents the functional density theory (DFT), as well as the ab-initio calculation method used in this context using the Castep calculation code which uses pseudopotential approximation (pp).

The last chapter presents in a first part the results of optimization of the calculations of the structural, electronic, elastic and anisotropy properties of XFeB4 (X= Y and Sc) without the pressure effect. The second part presents the XFeB4 (X= Y and Sc) calculation results under the traction pressure effect.

Finally, I end with a general conclusion which conclude all the main results of my work.

2 CHAPTER:RARE EARTH AND THEIR INTEREST METTALOIDS-TRANSITION METALS

2.1 Rare earth elements

2.1.1 What are the rare earth elements?

Chemical elements, such as carbon, hydrogen, and oxygen. Their atomic numbers range from 57 to 71. There are two other types (Y and Sc) due to their appearance in metals with elements of lanthanides, that have similar properties, sometimes attached to these elements. But the main rare earth elements are those fifteen. To prepare the first element, lanthanum, we start a barium seed and add one proton and one electron to it represented in (Fig-1-) and we add each additional element of the earth's successive protons an additional proton and an

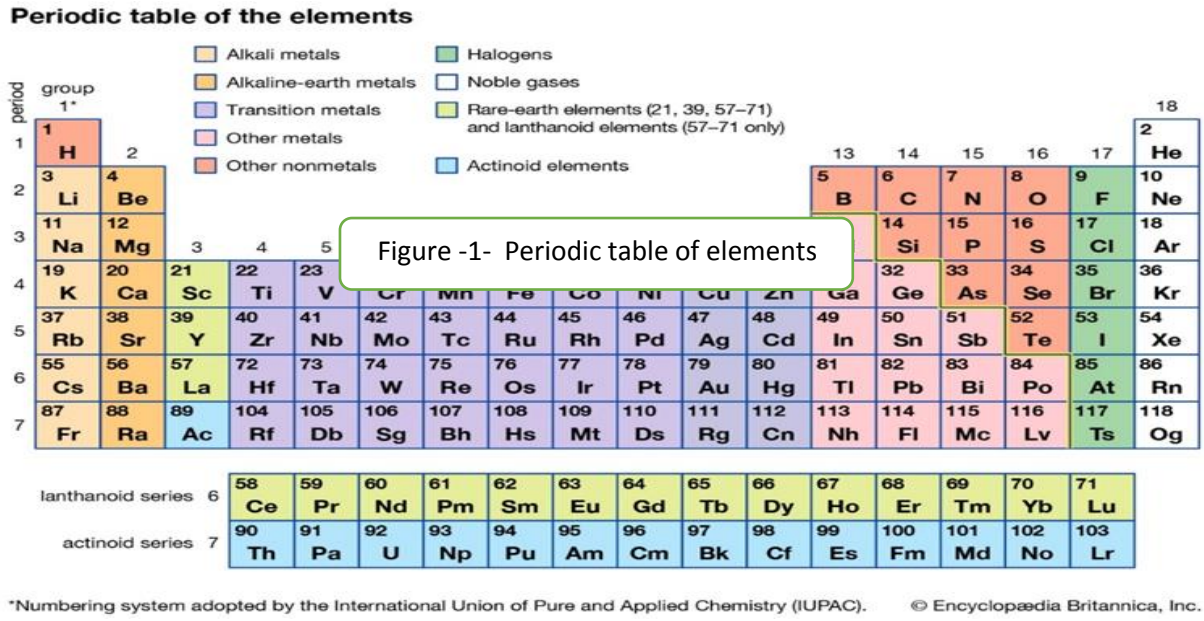


Figure -1- Periodic table of elements

electron [1].

2.1.2 Discovery and early history

The rare earth elements were known with the discovery of the black metal "etterbite" (renamed as Vadolinite in 1800) by Lieutenant Karl Axel Arthionis

in 1787, in a quarry in the village of Iterby, Sweden.

They are elements that were called ancientrare earth metals,

although not all of them are rare, as some of them are more

prevalent in nature than lead, and have retained this name even though they are classified today as the elements of the lanthanide, relative to the first elements of which are lanthanium La as it is sometimes referred to as the internal transition elements[1]. It was marked before the beginning of the nineteenth century with scarcity and high price, as it attracted the attention of only a few scientists, whose number did not exceed in the world at that time two hundred scientists, then the efforts gradually joined together, and attention increased to these soils to explore the depths of its elements on an experimental level in order to separate some of them On the one hand, it shows its physical and chemical properties, on the other hand [5].

2.1.3 Geographical distribution

China produced 95% of the rare items in 2010, and at the same time has 37% of the proven reserves. It was to impose export quotas in September 2009, with the ensuing declines to levels that did not meet global demand, and what appeared to be a Chinese ban on the export of rare earth metals in October 2010 due to an international incident with Japan that focused attention on other potential sources of these minerals. News analysis in the New York Times [8] showed that deposits of rare metals found in the United States, Canada, Australia, India, Brazil and elsewhere, are not exploited or at least not purified outside China, for environmental reasons represented in (Fig-2-)

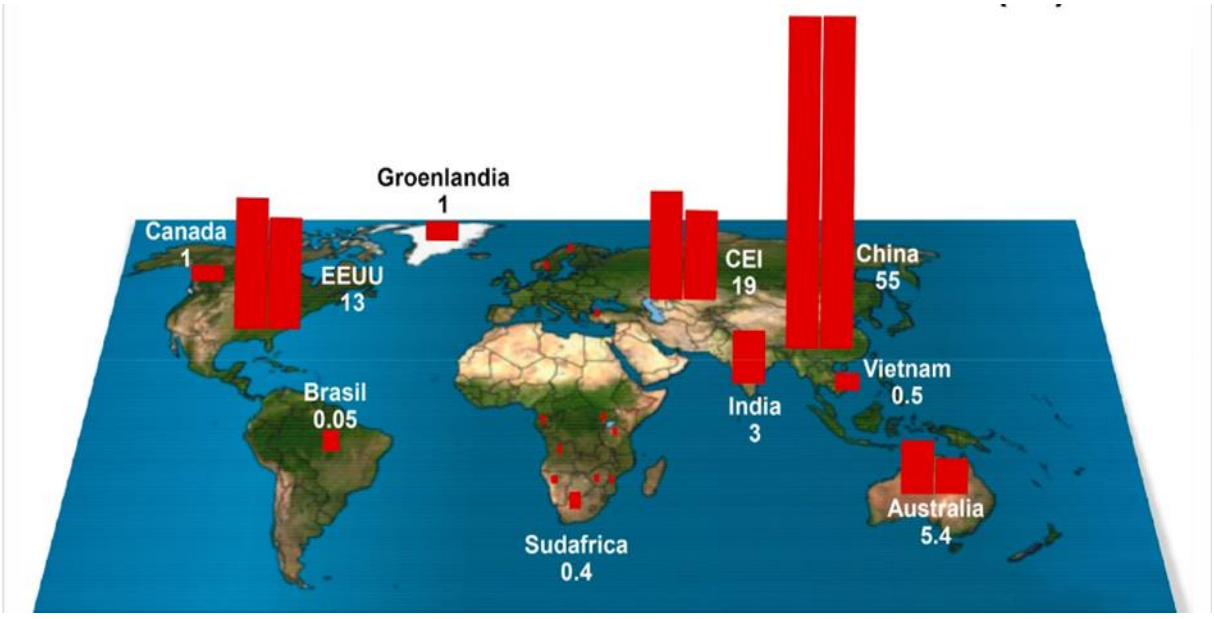


Figure-2- Geographical distribution of REE

2.1.4 Important elements for the manufacture of modern appliances

These elements are distinguished by a number of important physical and chemical properties that qualify them to enter into the manufacture of a large number of modern and advanced electronic devices, some of which have superior electrical conductivity at high temperatures, some are corrosion resistant and characterized by high hardness, and a number of them are used as excellent oxidizing agents that enter into some chemical industries, such as refining oil and its derivatives, and some rare elements are used as catalysts that are used to accomplish some chemical processes within a relatively short time and to the fullest extent.

The electronic composition of rare earth elements atoms plays an important role in highlighting some of the chemical and physical properties of them, as the electronic distribution of most of them is within the orbit of 4f, which plays an important role in giving them a number of unique properties [10].

These qualities enabled these elements to take center stage in the modern electronic devices industry since 1949, these elements have gained great importance when the European component produced from the "Mountain Pass" mine in California was used in the manufacture of the first television capable of broadcasting in color, but now these elements in the manufacture of laptops, digital cameras, smart mobile phones, flat-screen TVs, and the production of DVD discs, and a number of them are used in the manufacture of hybrid electric cars, miniature batteries and strong high-performance magnets that are used in the manufacture of electricity generating turbines from wind movement, and some of these elements are used to produce special types of lasers Also, these elements are of special importance in the field of manufacturing electric energy saving lamps and optical fibers cables and magnetic resonance imaging devices and satellites, while in the military field, rare earth elements are used in the manufacture of many military equipment, such as night vision goggles, precision guidance missiles, radar systems and communications advanced aviation and air navigation equipment some see (Fig-3-) [1 ,2].

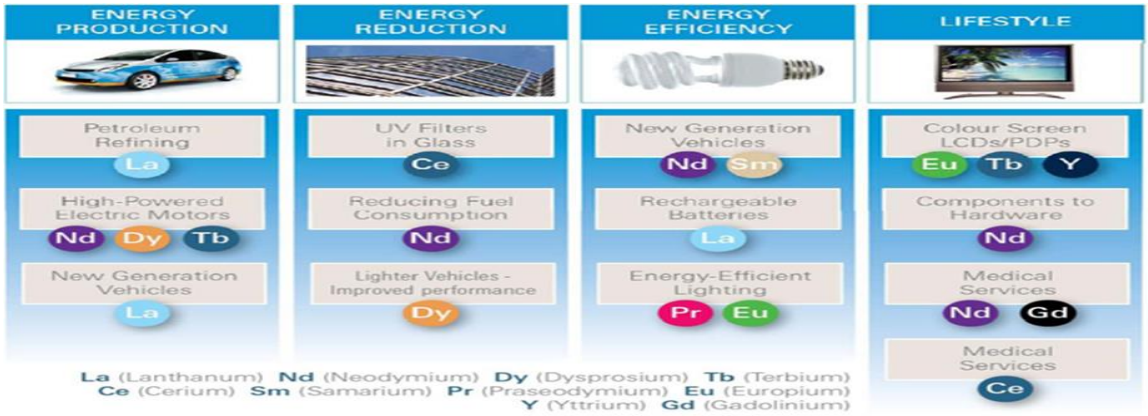


Figure -3- Applications of REE

2.1.5 Technical uses

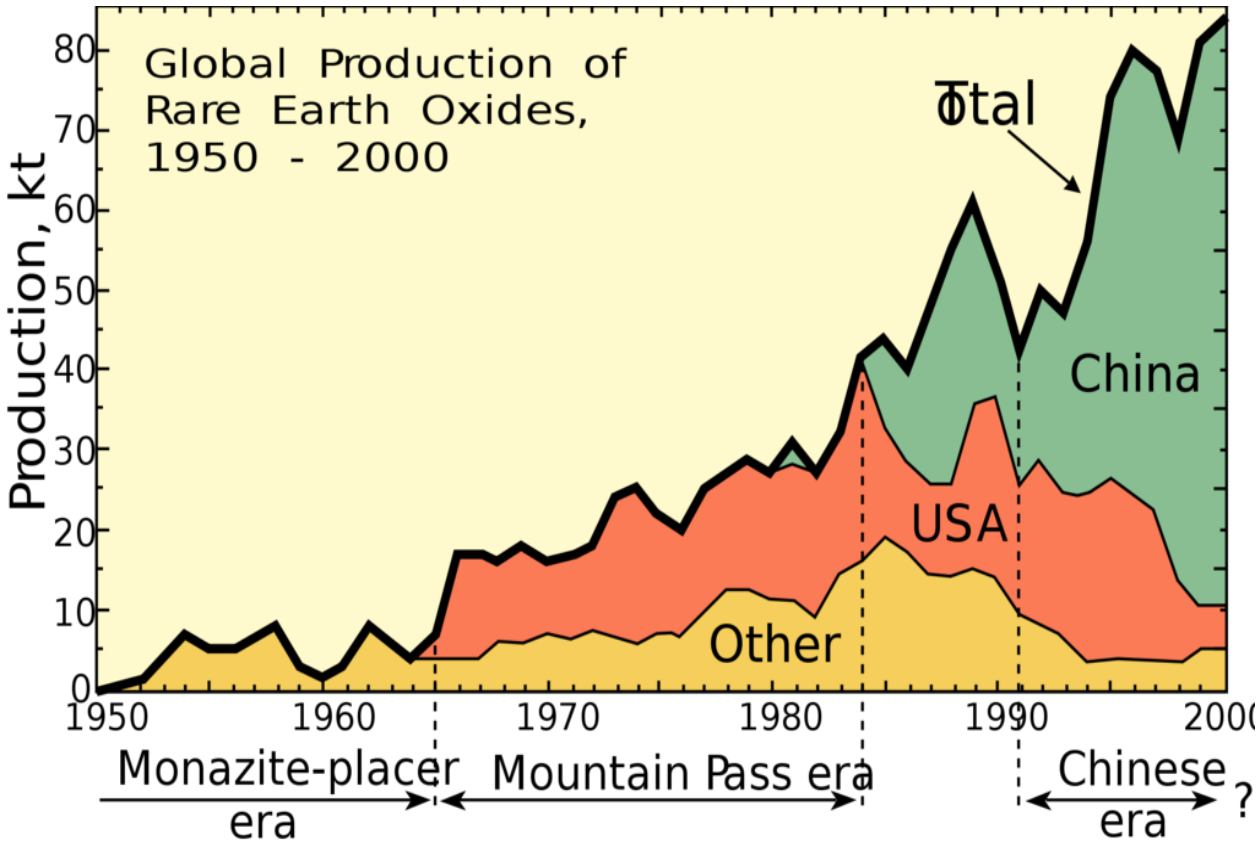
The rare elements differ in their physical and chemical properties, and the scandium element is one of the least rare elements in the atomic number. It was discovered in 1879 and is a transition metal element, white in color, that interacts with water and air, and scandium is used to produce alloys with aluminum for the manufacture of space vehicles and aircraft, as well as Scandium oxide is used in the manufacture of high-light bulbs [9].

As for the element yttrium, it is a silver transition metal, discovered in the year 1843 and used in the screens of cathode ray tubes, and in the production of a kind of industrial agate that filters microwaves and radar devices as it enters the manufacture of nuclear reactors due to its low interaction with neutrons.

2.1.6 The global production of the rare earth elements

Until 1948, most of the world's production of rare earth elements was from placer dust found in India and Brazil. In the fifties, South Africa became one of the countries of the world producing rare earth elements, after the discovery of a huge race of rare earth elements in its monazes. From the sixties until the eighties, the mountain pass for mining rare earth elements in California became the world's leading producer.

Today the reservoirs of India and South Africa still produce concentrates of trace elements, but they dwindle to Chinese production. China now produces 97% of the global production of RRE represented in (Fig-4-)[6,8].



2.2 The metalloids

2.2.1 What are metalloids

The elements are called semiconductor metals with conductors, due to their average electrical conductivity; As these substances fall between the conducting elements of electricity and dielectric elements, they are also classified in the category of crystalline solids, and one of their most important uses; It is used as a basic material in the manufacture of various types of electronic devices such as; transistors and integrated electrical circuits, as well as these devices of wide applications in practical life, due to the efficiency, quality and reliability of these devices, in addition to their low cost, and it is also possible to use these materials as independent components, and from their applications; energy and optical sensors and light emitters and others, and one of the characteristics of these materials is that they can handle high current and voltage, as they merge into very accurate and complex electronic circuits, and the metal-like have a promising future, due to the high demand in the local and global industries and markets[11].

2.2.2 Metalloids caracterstics

Metalloids elements are semiconductors at room temperature, in natural conditions, located between conducting elements and dielectric elements, but in the event of a temperature rise, their conductivity changes to become very close to the conductivity of minerals for electricity, and at low temperatures semiconductors are as insulating materials completely electricity, and this behavior has a good reason, which is the internal structure of it, as there may be a limited movement of electrons, depending on the crystal structure of the material used, and among the most important of those materials used; silicon, germanium and gray tin have been processed into conducting materials by incorporating some impurities into them, and the scientific explanation for this is that; when these materials are added, free electrons are added in these crystal structures to the original host materials, by attracting electrons[12].

2.2.3 History of metalloides

A metalloid is a chemical element whose properties are intermediate between those of metals and non-metals or are a combination of these properties. in the scientific literature, in the absence of a standard definition of metalloids, the list of elements classified in this family varies according to the authors.

The six elements generally recognized as metalloids are Boron 5B, Silicon 14Si, Germanium 32Ge, Arsenic 33As, Antimony 51Sb and Tellurium 52Te. Five others are less frequently classified as metalloids: Carbon 6C, Aluminum 13Al, Aelenium 34Se, Polonium 84Po and Astatine 85At. The latter, historically ranked among the halogens in the extension of the other elements of the 17th group, tends to be more considered as a metalloid as its chemical properties are better characterized. In a standard periodic table, they are distributed diagonally in the block p along the old line of demarcation between metals and non-metals represented on the periodic tables of the first half of the twentieth century represented in (Fig-5-).

13	14	15	16	17	18
5 **B** Boron 10.81	6 **C** Carbon 12.011	7 **N** Nitrogen 14.007	8 **O** Oxygen 15.999	9 **F** Fluorine 18.998	10 **Ne** Neon 20.180
13 **Al** Aluminum 26.981	14 **Si** Silicon 28.085	15 **P** Phosphorus 30.973	16 **S** Sulfur 32.06	17 **Cl** Chlorine 35.45	18 **Ar** Argon 39.948
31 **Ga** Gallium 69.723	32 **Ge** Germanium 72.630	33 **As** Arsenic 74.921	34 **Se** Selenium 78.971	35 **Br** Bromine 79.904	36 **Kr** Krypton 83.798
49 **In** Indium 114.82	50 **Sn** Tin 118.71	51 **Sb** Antimony 121.76	52 **Te** Tellurium 127.60	53 **I** Iodine 126.90	54 **Xe** Xenon 131.29
81 **Tl** Thallium 204.38	82 **Pb** Lead 207.2	83 **Bi** Bismuth 208.98	84 **Po** Polonium [208.982]	85 **At** Astatine 209.987	86 **Rn** Radon 222.018
113 **Nh** Nihonium [286]	114 **Fl** Flerovium [289]	115 **Mc** Moscovium [289]	116 **Lv** Livermorium [293]	117 **Ts** Tennessine [293]	118 **Og** Oganesson [294]

The metalloids have a metallic appearance but are fragile and poor conductors of electricity. Their chemical properties are essentially those of non-metals. They can form alloys with metals they generally have too low a mechanical resistance to be able to be used in structural applications, and are generally used through their alloys, like catalysts, in fireproofing, in the manufacture of glasses, the optical disc drives, optoelectronics, pyrotechnics , semiconductors and electronics. It was the properties of Germanium and Silicon that led to the emergence of the semiconductor industry in the 1950s and the development of solid state electronics in the early 1960s[12].

2.2.4 The properties of metalloids elements

The semi-metallic elements are characterized by the difficulty of passing them to the electrical current through the material, as their resistance decreases as the temperature increases. Exactly what he wants to make of these metal-like pieces; The metal increases its resistance while the metal resemblance decreases its resistance when the temperature rises, and therefore the electric current flows easily and in an optimal way. Another characteristic of these materials is that when adding any impurities to these crystalline structures, the electrical current is prohibited or it may be redirected on purpose, so it is granted that these materials have sufficient ability to control how and how much electrical currents pass, and these properties are also available in silicon; not only is it plentiful and easy to handle, it is strong and connected to electricity in a very good controlled manner[13].

2.3 Transition metals

2.3.1 Definition

Transitional elements express the chemical elements that carry a valence electron; The concept of valence electron refers to the electron that can participate to form chemical bonds with two structures instead of one, and the word transitional explains the similarity between the atomic structure and the resulting properties of the specific elements; As it does not have chemical significance in itself,[12], all transitional elements are involved as metallic elements; As it includes the most famous elements in the periodic table, including Gold, Iron, Silver, Copper, Mercury[12].

2.3.2 Discovery of the transitional elements

Iron is one of the most transitional elements present in the earth's crust, as it is the fourth most present element among all other elements, and the second after Aluminum is between the mineral elements in the earth's crust, and there are also some important transitional elements such as Tungsten, Platinum, Gold, and Silver are found in small quantities in the crust The transitional elements [12] were known as iron, copper, silver, and gold in ancient times, and in the early eighteenth century the rest of the transitional elements were discovered, and Rhenium, which is the most recent transitional element discovered in 1925 between platinum ores.[12].

2.3.3 Characteristics of transitional elements

The transitional elements are distinguished as metallic, which is the prominent similarity between all twenty-four transitional elements, most of which are characterized by rigidity, strength, and luster [12]:

- Characterized by their boiling point, melting point
- Good conductors of heat and electricity
- Distinguished by their flexibility; Therefore, it is easy to knock, shape and fold.
- Have little ionization energy.
- Most of these elements dissolve with mineral acids.

2.3.4 The importance of transition metals

Their importance is due to their ability to form complex that are distinguished by[14] :

1 -Radius is small.

2-Her positive charge is high.

3 -It has empty orbits of sufficient energy to receive

4- Electron pairs are coordinated group.

2.3.5 Magnetic properties

It has magnetic properties, and in particular, magnetic bars.

Paramagnetic substance: it is the material that attracts to the magnetic field This is due to the presence of orbits f, d that are not filled with electrons, which leads to the presence of individual electrons

Most of them dissolve in dilute mineral acids, some of which do not affect these acids like Gold and Platinum[14].

2.3.6 Arrangement of transition metals

All transitional elements form stable bonds in one or more of the basic oxidation states. Arrangement of the transitional elements represented in (Fig-6-) .The transitional elements may be divided according to the structure of the electrons in the atom via three basic transition chains where the first major main chain begins with Cassium, or Titanium, and ends with an element Zinc, the second chain contains the elements of Yuetrium and Scadmium, while the third chain extends from the element Lanthanum to Mercury, and these basic

transition chains are among the group of thirty, which are sometimes called elements of the transitional block D[14].

(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)
21 Sc 44.95591	22 Ti 47.867	23 V 50.9415	24 Cr 51.9961	25 Mn 54.9380	26 Fe 55.845	27 Co 58.93320	28 Ni 58.6934	29 Cu 63.546	30 Zn 65.409
39 Y 88.90585	40 Zr 91.224	41 Nb 92.90638	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.90550	46 Pd 106.42	47 Ag 107.8682	48 Cd 112.411
	72 Hf 178.49	73 Ta 180.9479	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.219	78 Pt 195.078	79 Au 196.96655	80 Hg 200.59

Figure-6- Arrangement of transition metals in periodic table

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3 Chapter. 2

Principles of density functional theory (DFT)

In this chapter, we will present a set of different methods or approximations used in calculating the different properties of solid bodies, depending on the functional theory of density, as the theoretical aspect Hohenberg. After this we will provide a special explanation of the cohen and sham equations used in the work as well as the importance of coding exchange and association with different types of functions such as (LDA , GGA…)

3.1 The schrodinge's equation

The Schrödinger equation is the starting point for all quantitative studies of the quantum system of crystals. The interacting particle system (ions + electrons) is described by the following Schrödinger equation [8] :

$$\hat{\mathrm{H}}\psi = E\psi \tag{2-1}$$

Where: **Ψ** is wave function, **H** is the Hamiltonian, **E** represents the system power.

The total Hamiltonian of the system is composed of the kinetic energy of all the particles and the energy of the interaction between them. When it's necessary the energy of interaction with the outer medium when the outer field is absent, the Hamiltonien wrote like that:

$$\hat{H} = \hat{T} + \hat{V}$$

$$\mathrm{H=Te + Tn + Ve\text{-}e + Vn\text{-}n + Ve\text{-}n} \tag{2-2}$$

(Te, Tn). The first two terms are the kinetic energy of the electrons and the nuclei respectively.

the last three limits are the potential energy effects of an electron-electron reaction; a nucleus-nucleus and an electron-nucleus

$$H=\sum_{i=1}^{N}\frac{-h^2}{2m_e}\Delta i+\sum_{i=1}^{n}\frac{-h^2}{2M}\Delta i+\frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\vec{r}_i-\vec{r}|}+\frac{1}{2}\sum_{\alpha\neq\beta}\frac{z\alpha z_\beta e^2}{|\vec{R}\alpha-\vec{R}_\beta|}-\sum_{i,\alpha}\frac{Z\alpha e^2}{|\vec{r}_i-R\vec{\alpha}|} \tag{2-3}$$

Transactions i and j are for electrons, and α and β coefficients are for the nuclei,

The masses of electrons and nuclei, respectively, m, M

Nuclei charge. Z α e

The distance between the two nuclei α and β $|\vec{R}\alpha - \vec{R}_\beta|$.

The distance between the nucleus α and electron i $|\vec{r}_i - \vec{R}\square|$. ²

The distance between the two electrons i and j $|\vec{r}_i - \vec{r}\square|$

3.2 Born-oppenheimer's approximation

This approximation assumes that the nucleus is static with respect to the electron, due to the very fast movement of electrons in relation to the nucleological movement of the kinetic energy of the nuclei with no movement in front of the electrons $T\mathrm{N} \cong 0$

The reaction energy between the nuclei is constant V_{NN} = cte, that is, the total Hamiltonian becomes the following formulation[9] :

$$\mathrm{H_e} = \mathrm{T_e} + \mathrm{V_{e-e}} + \mathrm{V_{e-}}\square \tag{2-4}$$

H*e* named electrons hamiltonien so

$$H_e = \sum_{i=1}^{N} \frac{-h^2}{2m_e}\Delta_i + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\vec{r}_i - \vec{r}\square|} - \sum_{i,\alpha}^{n}\frac{Z\alpha e^2}{|\vec{r}_i - \vec{R}\alpha|} \tag{2-5}$$

The Schrödinger electron equation $H\Psi_e = E\Psi_e$ (2-6)

3.3 Hartrie-Fock

This approximation depends on the independent electron model, where Hartree assumed that each electron moves individually in the intermediate field generated by the nuclei and the rest of the other electrons (the free electron model), and thus our problem becomes changed from a large number of electrons to a single electron, and Hamilton writes the sentence with [3-10] :

$$H = \sum_{i=1}^{N} H_i$$

$$\left[\frac{-h^2}{2m}\nabla^2 + U_i(\vec{r_i}) + V_i(\vec{r_i})\right]\psi_i(\vec{r}) = E\psi_i(\vec{r}) \tag{2-7}$$

$U_i(\vec{r_i}) = \sum_k \frac{Z\kappa\ e^2}{|r_i - R^\circ\kappa|}$ it represents the potential energy of the electron i in the nucleus field k

R_K Represents the position of the nucleus

The effective potential of Hartree

$$V_i(\vec{r}_i) = V_H(\vec{r}_i) = -\int dr' \rho(\vec{r}') \frac{1}{|\vec{r}_i - r'|} \quad (2\text{-}8)$$

$$H_i = -\frac{h^2}{2m}\Delta_i + V_{eff}(r_i) \quad (2\text{-}9)$$

Effective latency can be expressed as the sum of these distributions by this relation:

$$V_{eff}(r) = V_H(r_i) + V_{ex}(r_i) \quad (2\text{-}10)$$

By compensation in Schrödinger equation:

$$[\frac{-h^2}{2m}\Delta_i + V_{eff}(r)]\Psi_i(r) = \varepsilon_i \Psi_i(r) \quad (2\text{-}11)$$

In 1930 Fook clear up that the wave function of Hartree did not respect the principle of Pauli exclusion so he entered the spin system so that there is an n probability for placing n electron at n position ($\overrightarrow{r_1}$, $\overrightarrow{r_2}$, ... $\vec{r}$) [11].

Schrödinger's equation after Fook's correction is written in the following statement

$$\frac{-\nabla^2}{2m}\Psi_i(\vec{r}) + V_i(\vec{r})\Psi_i(\vec{r}) + V_H(\vec{r})\Psi(\vec{r}) - \sum_j \int \frac{dr}{|\vec{r} - \vec{r}'|}\Psi(\vec{r}')\Psi_i(\vec{r}')\Psi(\vec{r}) = E_i\Psi_i(\vec{r}) \quad (2\text{-}12)$$

The threshold that made the difference between a Hartree approximation and a Hartree Fock approximation is the latency of the exchange given:

$$V_x = -\sum_j \int \frac{dr}{|\vec{r} - \vec{r}'|}\Psi(\vec{r}')\Psi_i(\vec{r}')\Psi(\vec{r}) \quad (2\text{-}13)$$

3.4 Density Functional Theory (DFT)

The density functional theory (DFT) is presently the most successful (and also the most promising) approach to compute the electronic structure of matter[12].

• In its original formulation, the density functional theory provides the ground state properties of a system, and the electron density plays a key role[12].

•The main goal of the density function is to predict the bonding bonds between atoms based on the principles of quantum mechanics [12].

In 1927 Thomas and Fermi gave a model that density can be relied upon to calculate kinetic energy

The results were weak to neglect the association between electrons

In 1964 Hohenberg and Kohen demonstrated that densities can be used to calculate system properties

The first Hohenberg-Kohn Theorem

Depends on taking the total energy of the system of the interacting electrons in an external potential (nucleus V_{ex} potential) is a single function of the density of the electron [1]. E=E(ρ)

The second Hohenberg-Kohn Theorem

The density of the electrons in their basic state is itself the lowest value of the energy of the system [1].

$$E(\rho_{\circ}) = MinE(\rho)$$

$\rho_{\circ}$ the density in the basic state

3.5 Kohn –Sham

Their idea was summed up by converting the total of the interacting electrons within the real latency into a virtual unreacted sentence in which the electrons move within the Kohn – Sham potential created by all nuclei and other electrons and have the same density that is found by means of a self-consistent solution to a set of Schrödinger's equations[14] :

$$H_{KS}\psi_i = E_i\psi_i$$

$$\left[\frac{-h^2}{2m}\nabla^2 + V_{io}(\vec{r}) + V_H(\vec{r}) + Vxc(\vec{r})\right]\psi_i(\vec{r}) = \varepsilon\psi_i(\vec{r}) \qquad (2\text{-}14)$$

$\psi_i(\vec{r})$ electron i wave function

$V_{io}(\vec{r})$ Nucleus latency

$V_H(\vec{r})$ Hartree latency

Where:

$$V_H(\vec{r}) = \int \frac{\rho(\vec{r}_1)\rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_1 d\vec{r}_2 \quad (2\text{-}15)$$

The active system of unreacted electrons in an active potential that is the potential of the real system is

$$V_{eFF} = V_H + Vxc + V_{ex}(r_i) \quad (2\text{-}16)$$

V_H Hartree Latency given by : $dr' \int \frac{\rho(r')}{|r-r'|}$

V_{ex} and V_{io} necleus latency

Vxc Latency of exchange and correlation given :

$$Vxc = Vx + Vc \quad (2\text{-}17)$$

Where: $Vxc(\vec{r}) = \frac{\partial Exc[\rho(\vec{r})]}{\partial \rho(\vec{r})}$

Thus, the Kohen Sham equation can be written as follows :

$$H\psi_i(\vec{r}) = [\frac{h^2}{2m}\nabla^2 + Ve_{FF}(\vec{r})]\Psi_i(\vec{r}) = \varepsilon\Psi_i(\vec{r}) \quad (2\text{-}18)$$

$$Ve_{FF}(\vec{r}) = V_{ex}(\vec{r}) + \int \frac{1}{|\vec{r}_i + \vec{r}|}\rho(\vec{r})d\vec{r} + Vxc(\vec{r}) \quad (2\text{-}19)$$

3.6 Approximations

Local density approximation(LDA)

This approximation was proposed by kohen and Cham in 1965 and the heterogeneous electron system was considered as a homogeneous system locally, that is, it only depends on the value of the electronic density at every point in space and the energy of the exchange is written - correlation with the following equation [2] :

$$E_{XC}^{LDA}(\rho) = \int \rho(r)\mathcal{E}_{XC}^{LDA}(\rho(\vec{r}))dr^3 \quad [5]$$

Note that the energy of exchange-correlation is divided into two parts

$$\mathcal{E}_{XC}^{LDA}(\rho) = \mathcal{E}_{X}^{LDA}(\rho) + \mathcal{E}_{C}^{LDA} \quad [6]$$

Generalised gradient approximation (GGA)

This approximation is a correction to the approximation of the density of the position as it exceeds it in accuracy $\rho(r)$ adds to its considerations the changes in the density of electrons $\nabla(\rho)$[13] (via the gradient of the electronic density). The phrase energy is written as follows [3, 4]

$$E_{\mathrm{XC}}^{GGA}(\rho\uparrow(\mathrm{r}),\rho\downarrow(\mathrm{r}))=\int\rho_{\mathrm{XC}}^{GGA}(\rho(\vec{r}),\nabla\rho(\vec{r}))dr^3 \quad [7]$$

$\nabla\rho(\vec{r})$ Expresses the gradient of electronic density

2.7.The pseudo –Latency method

Is a method designed to simplify the calculations, mainly relying on reducing the system (nuclei total electrons) to a system (related to valence electrons) in a false potential consisting of the nuclei of the nuclei and the quantum of the inner electrons (highly related), however the calculation is determined in fact, this approximation is well explained by the fact that the inner orbitals have a low energy that is expected soon from, as they are less sensitive with the medium and do not participate in any chemical bonds and are difficult to represent in the base of the nucleus, because they have strong vibrations around the nucleus. A sufficiently less predictive view that extends away from the nucleus. It defines primarily physical and chemical properties.

The basic idea was put forward by Fermi in order to simplify the calculation of electronic structures by canceling internal or cardiac cases.

The effect of the inner electrons has been replaced by an effective false potential, which is equivalent to replacing an external potential (electron-nuclei) with a very weak potential[15].

2.8.CASTEP: Cambridge Serial Total Energy Package

It is a specialized program in the field of quantum mechanics and depends on a theoretical study within the framework of the function of density using the method of pseudo-potentials to simulate the properties of solid objects as well as the surfaces of a large number of DFT and allows the extraction of electronic, structural, materials such as ceramics, semiconductors as well as minerals, light and others without the need to doing a real

experiment or rather it can be said that the castep performs virtual digital experiences. In the field of the theory of condensed matter. The Castap program has several versions of CDG that were developed by a group.

Castep code: we use some parameters as:

• The pseudopotential approximation,

• K-points

• Energy cutoff (E_{cut})

The pseudo potential: is an attempt to replace the complicated effects of the motion of the core electrons of an atom and its nucleus with an effective potential.

k-points: meaning: they are sampling points in the first Brillouin zone of the material.

The Cutt- OFF Energy: tells us about the cutoff on the number of plane wave functions being utilized as basic functions to represent the wave function. Theoretically, an infinite number of basic functions is required to produce an exact answer. However, this is not computationally practical and a cutoff must be introduced.

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4 Chapter 3

Results and discussion

4.1 Introduction

I use ab-initio calculation for the structure, electronic, hardness and anisotropies elastic properties of $YFeB_4$ and $ScFeB_4$ compounds. Mechanical anisotropies are discussed by the plot of the three dimensional (3D) surfaces and planar contours of Young and bulk modulis of rare earth compounds study at several crystallographic planes, ((100), (010) and (001)) to reveal their elastic anisotropy.

4.2 Computational details and structural optimisation

The use of computer simulation techniques has become more important in understanding the physical properties of compounds Total energy calculations are performed within density functional theory (DFT) [1] using CASTEP code [2] for the whole study which uses the plane wave expansion method in reciprocal space[3]. The generalized gradient approach approximation (GGA), proposed by Perdew-Burke-Ernzerhof (PBE) was used for exchange-correlation energy calculations [4].The Ultra-soft Vanderbilt pseudo-potentials are employed to represent the electrostatic interactions between valence electrons and ionic cores [5] which are used with the following valence electronic configurations for the interaction between the (electron and ions) where the Fe orbits ($3d^6$ $4s^2$) and Sc ($3s^2 3p^6 3d^1$ $4s^2$) and B ($2s^2.2p^1$) and Y ($4d^1$ $5s^2$) are treated as valence electrons. Brillouin region samples were taken using an 8 x 8 x 8 group of Monkhorst-Pack mesh atomic positions comfortable and light mated with a density mixing scheme. The improved crystalline structures of $XFeB_4$ (X = Y and Sc) in the orthorhombic structure (space group: 55 Pbam) as shown in (Fig-1-). The network parameters (a, b, c), are listed in Table-1- along with available experimental data for comparison

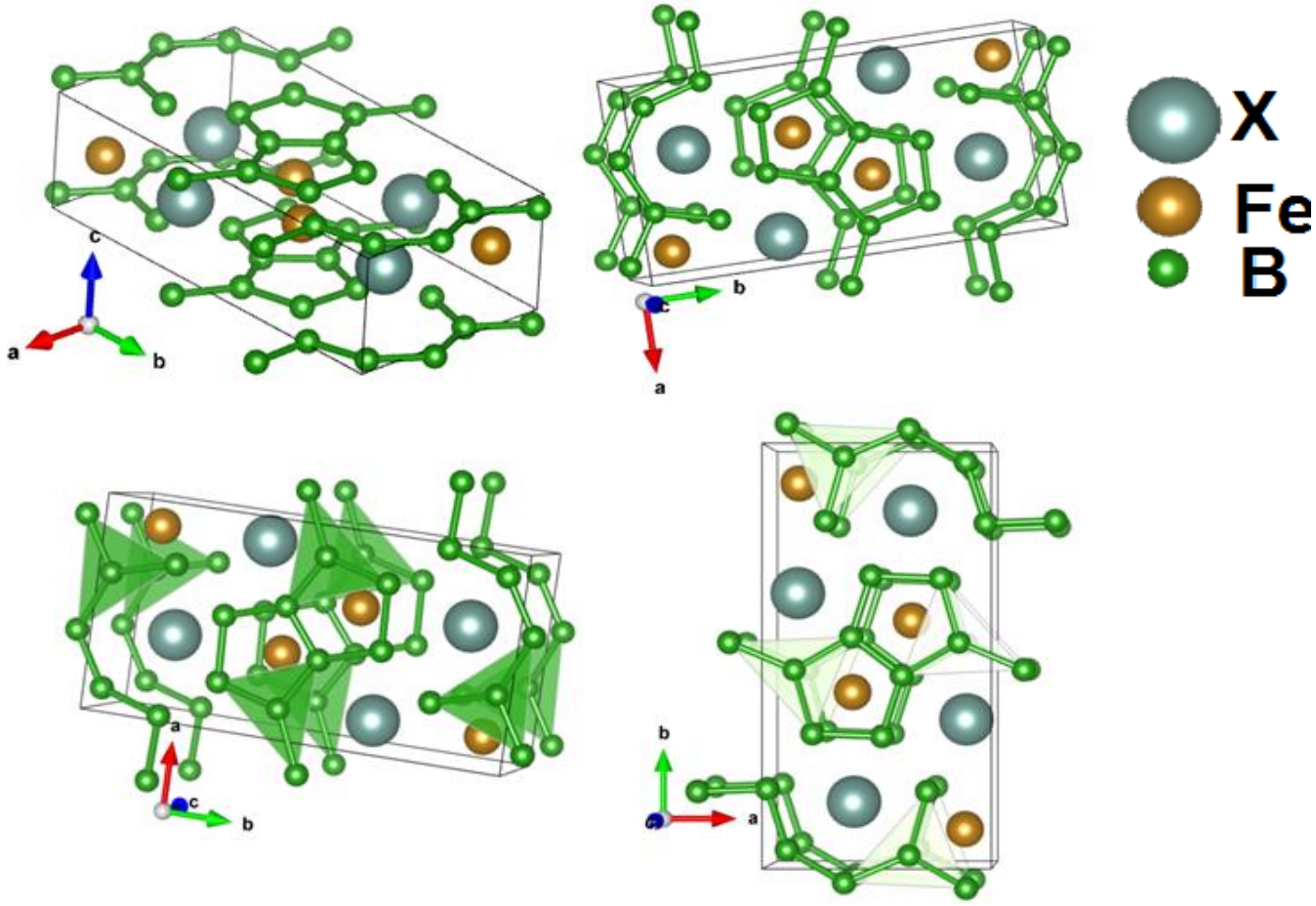


Figure.1. Crystal structure of XFeB4 (X=Sc, Y) illustrated by ball and stick model and the metal transition, boron atoms environment.

Table 1.The network parameters (a, b, c) for XFeB4 (X= Y and Sc)

Compounds	a	b	c	Atomic position
YFeB4	5.89	11.39	3.42	Y 0.373000 0.150000 0.500000
				Fe 0.3670000.412000 0.500000
				B1 0.024000 0.19000 0.000000
BEFORE				B2 0.111000 0.0460000.000000
				B3 0.139000 0.4680000.000000
				B4 0.218000 0.317000 0.000000
YFeB4	5.95	11.53	3.40	Y 0.374797 0.151304 0.500000
				Fe 0.368538 0.4140870.500000
				B1 0.024064 0.1884000.000000
AFTER				B2 0.1099470.0450240.0000000
				B3 0.1412500.4679640.0000000
				B4 0.221088 0.3178140.000000
	5.91^{exp}	11.40^{exp}	3.41^{exp}	
ScFeB4	5.89	11.39	3.42	Sc 0.373015 0.150027 0.500000
				Fe 0.366545 0.411541 0.500000
BEFORE				B1 0.025413 0.192280-0.00000
				B2 0.113986 0.047123 0.00000
				B3 0.135781 0.468569 0.000000
				B4 0.215183 0.315193 0.000000
ScFeB4	5.75	11.10	3.20	Sc 0.371366 0.149849 0.500000
				Fe 0.366034 0.4110770.500000
AFTER				B1 0.022759 0.193396-0.000000
				B2 0.113710 0.047717 0.000000
				B3 0.135397 0.468766 0.000000
				B4 0.212009 0.314664-0.000000

^{exp} Ref article: Abdullah Candan et al 2019 Phys. Scr. 94 125710

4.3 Density of state (dos)

Total densities of state DOS and PDOS for $XFeB_4$ compounds are illustrated in (Figure-2-) and (Figure-3-) The most obvious feature of $XFeB_4$ compounds is that they are conductor, since the d bands of Fe and Y which are raised above the Fermi level, this overlap prove that our compounds are conductor. It can be seen that the total DOS is dominated by the density of d electrons of iron and by a few d electrons of Yttrium, also strong hybridization d-p of electrons of Fe-B at the Fermi level was observed, this hybridization take magnetic moments to be zero, On this basis, the difference between density spin up and spin down are mirror, which make the magnetic moment equal zero. There are several naturally occurring magnetic elements: iron, nickel, and cobalt. By introducing these into a material, they can introduce favorable magnetic properties in a material, as they can lose their magnetic moment, following the above arguments of hybridization between Fe-B, our materials lose their magnetic moments represented in (Fig-5-).

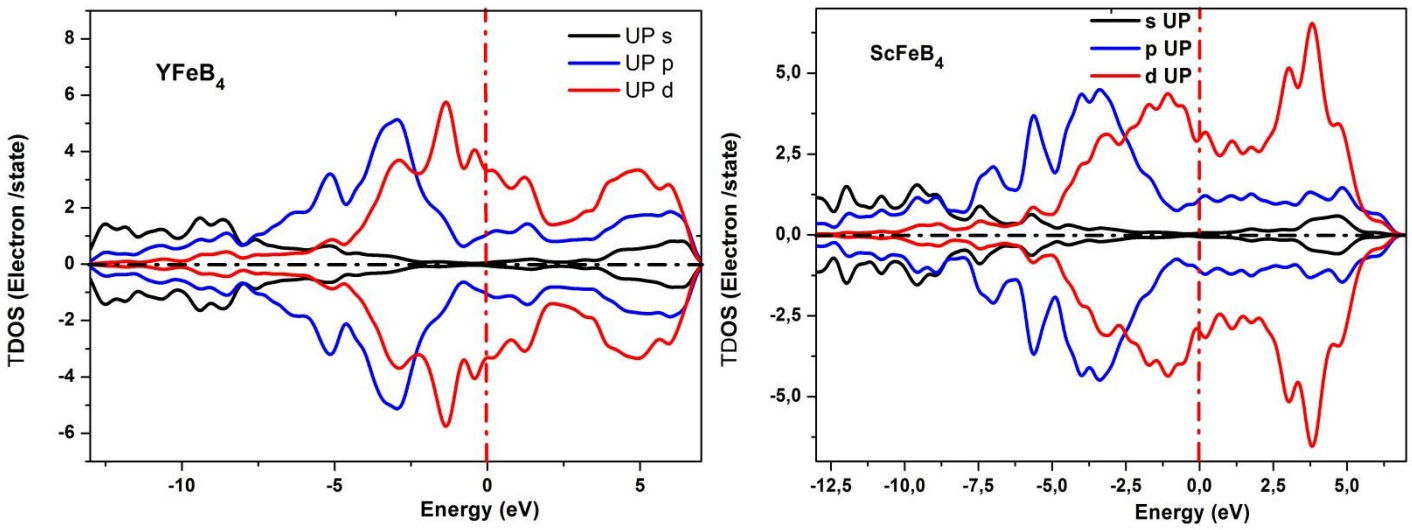


Figure-2-. The calculated total DOS of $XFeB_4$. Dashed line represents the Fermi level.

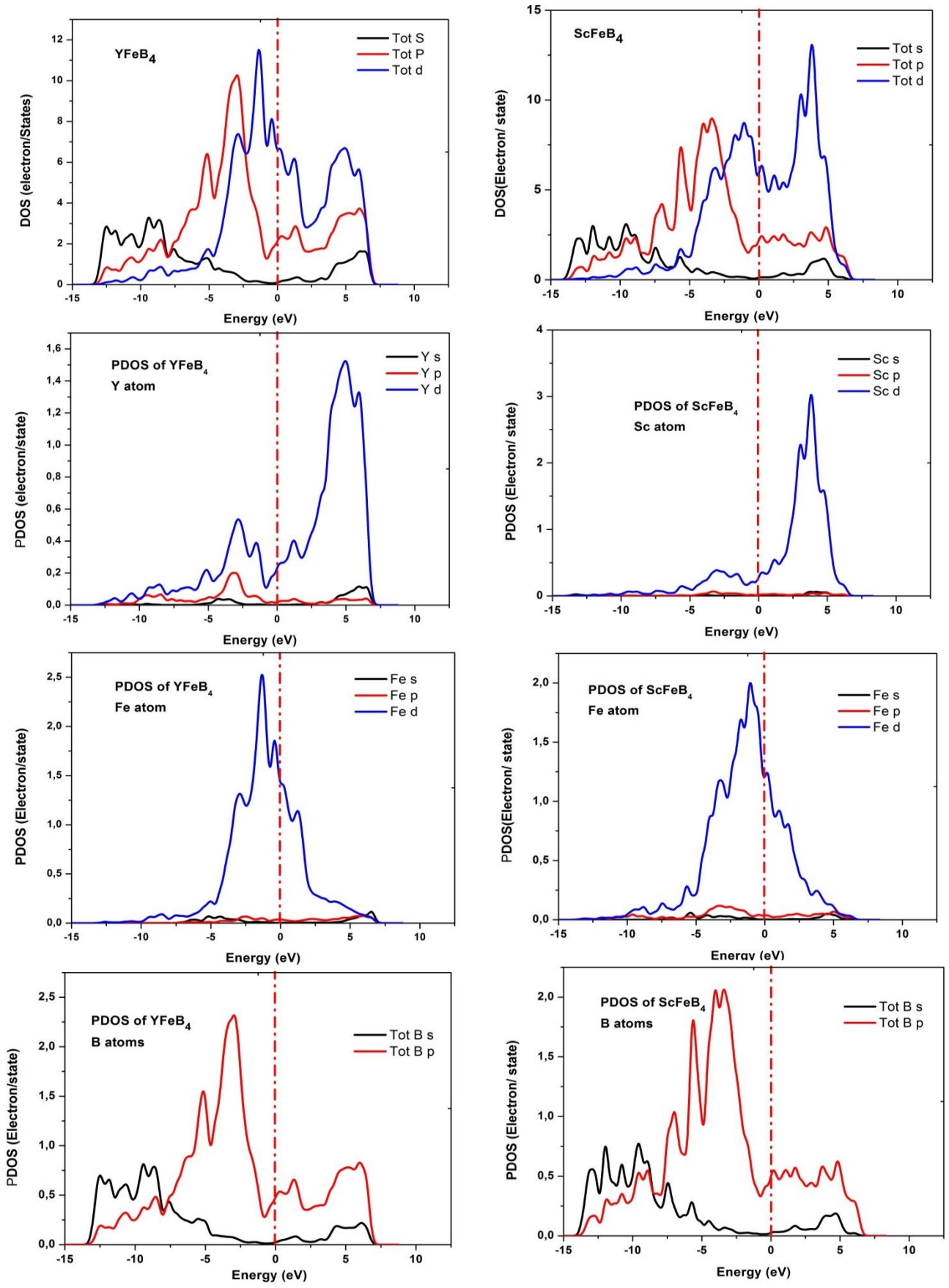


Figure-3-. The calculated total and partial DOS of XFeB4. Dashed line represents the Fermi level.

The strong interaction between B atoms causes a 2s-p hybridization (Figure-4-) and leads to strong covalent bonds. It is clearly shown that there exists an even stronger bond (zigzag chains) between B atoms in x and y direction. It is this strong covalent bond which makes the B atoms form linear zigzag chains in $XFeB_4$ and make our materials stronger (see later $C_{22}>C_{11}>C_{33}$)

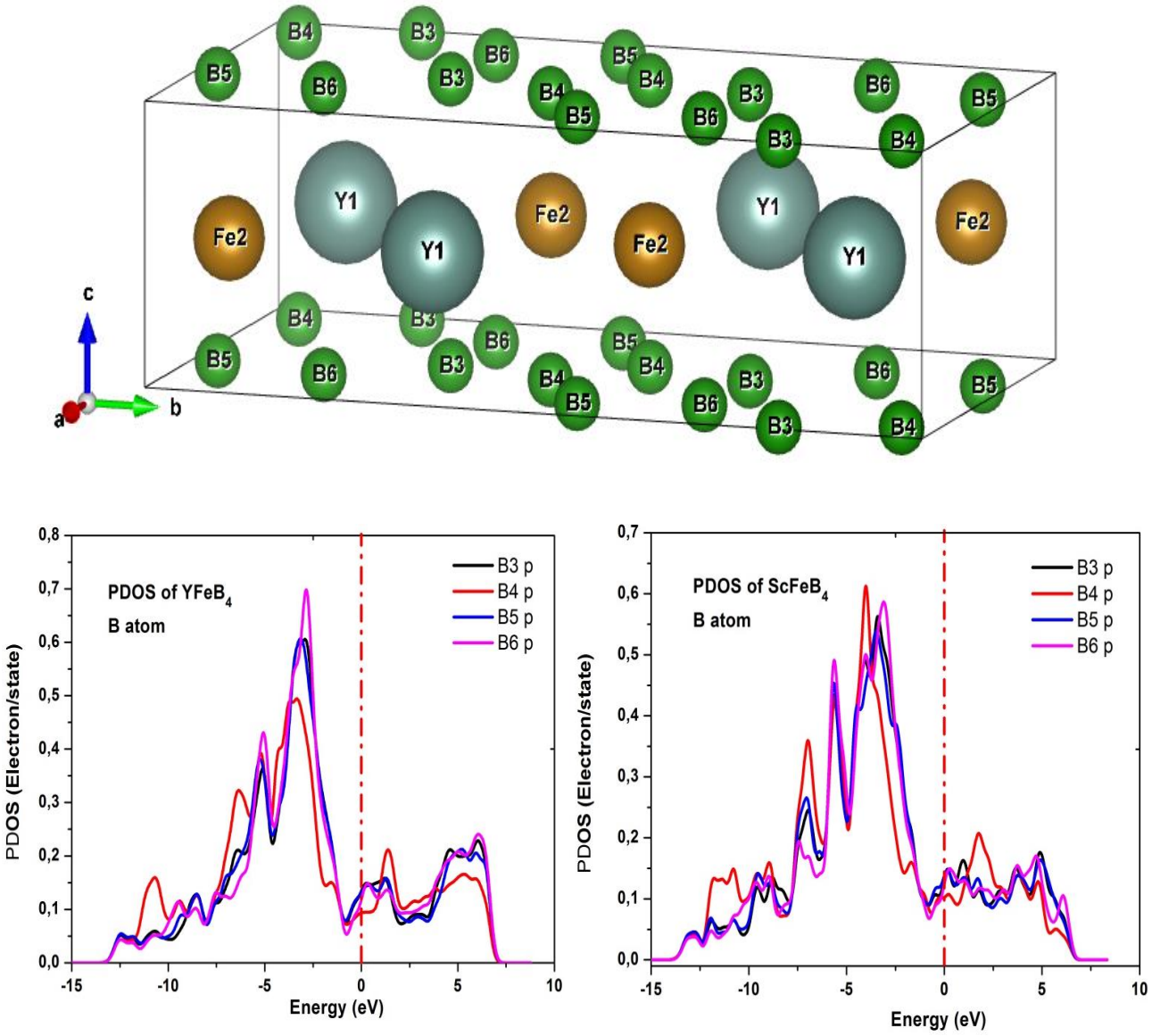


Figure -4- Hybridation of B atomes

4.4 Population analysis

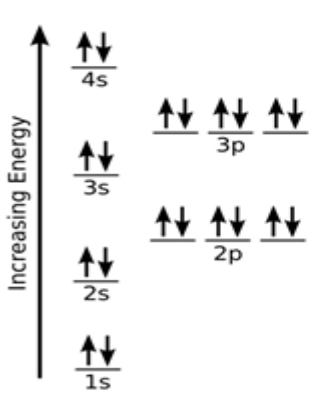
Mulliken population analysis (MPA)[20] is a method for calculating partial atomic charges based on the population of linear combined atomic orbitals (LCAO) bases. This is implemented in CASTEP by Segall *et al*[21]. based on the method of Sanchez-Portal [22] which provides the link between methods using LCAO and those using plane waves. MPA method is applied to overlap population and bond length between atoms. I calculate the average bond length (A):

Table-2-. Average bond length of nearest-neighbor atoms

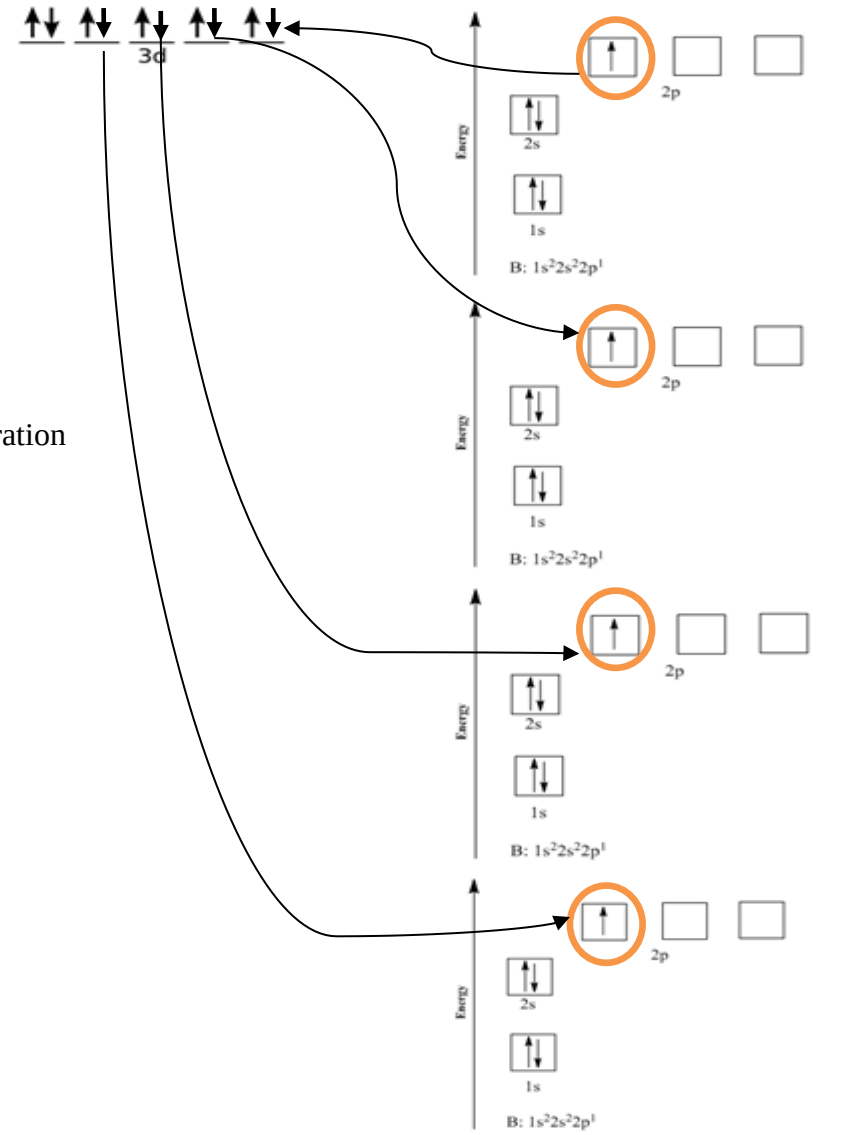
Compound	Bond length (X= Y , Sc)					
	B-B	Fe-B	Fe-Fe	X-X	X-B	X-Fe
$YFeB_4$	1.785255-2.823872	2.283057273	>3	>3	2.692835714	>3
$ScFeB_4$	1.728435-2.79136	2.174664	>3	>3	2.556447143	>3

4.5 Pauli exclusion principle and Hund rule

Pauling was one of the founders of quantum chemistry. His contributions to the theory of the chemical bond include the concept of orbital hybridization, and the Pauli exclusion principle is; if two electrons reside in the same orbital, thus the electrons must have opposite half-integer spin projections of 1/2 and −1/2, add to Hund rule that if two or more orbitals of equal energy are available, electrons will occupy them singly before filling them in pairs, by those principle we can justify the hybridization between iron atoms and Boron atoms (see figure below)



Iron (Fe) electron configuration

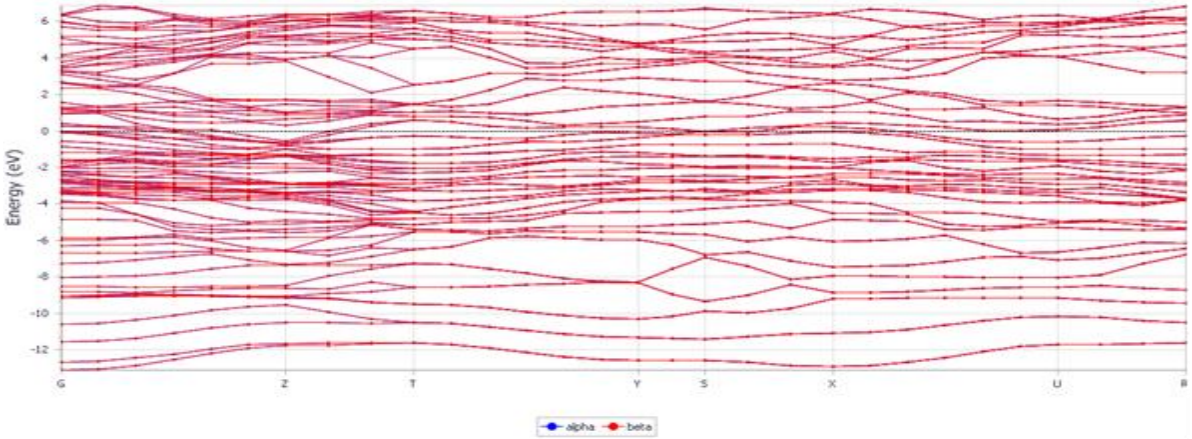


Boron (B) electron configuration

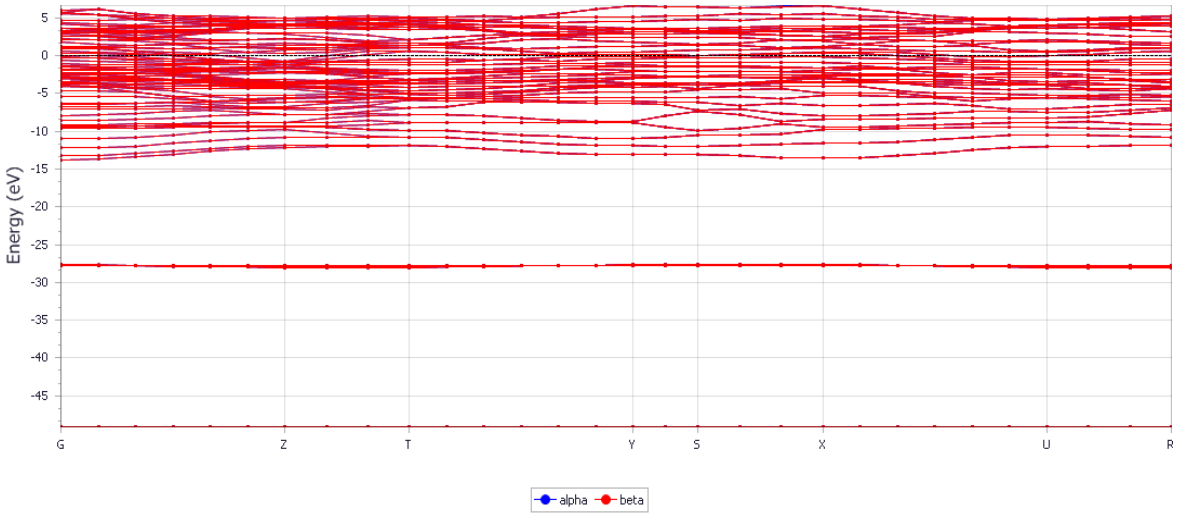
Figure-5-. Hybridization between Fe-B

4.6 Band stucture of xfeb4

Band structure of XFeB4, shows that there is an overlapping of the valence band and the conduction band, confirming the conductor nature of structures under normal conditions. The bands just above the Fermi energy are due to the empty 3d states of rare earth elements, and transition metals (Y, Sc and Fe) Figure-6



Bande structure of $YFeB_4$



Bande structure of $ScFeB_4$

Figure-6- The calculated band structures for $XFeB_4$ compound near Fermi level

4.7 Mechanical properties

To understand bonding type, ductility (or brittleness) and mechanical stability of a crystal, elastic constants (Cij) could be calculated. The elastic constants (C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, and C_{23} for orthorhombic structure) at 0 GPa and 0 K are successfully obtained by using the Castep program and the results are listed in Table-1-. As can be

Table 3. The calculated full set elastic constants of $XFeB_4$ YXB_4 (X = Y and Sc).

Compounds	C11	C12	C13	C23	C22	C33	C44	C55	C66
YFeB4	522.79	133.12	124.65	122.43	527.14	376.66	170.19	151.86	209.28
	505.9[a]	74.10[a]	85.90[a]	94.98[a]	505.35[a]	386.06[a]	229.3[a]	173.5[a]	177.9[a]
ScFeB4	530.57	118.85	92.02	104.50	546.02	423.23	184.10	186.84	249.12

[a] Ref article: Abdullah Candan et al 2019 Phys. Scr. 94 125710

concluded from table 3, $XFeB_4$ (X = Y and Sc)

Generally, the elastic constants C_{11}, C_{22} and C_{33} are very high, which indicates the high resistance to the axial compression in these directions. Moreover, it is shown in table -3-that the elastic constants C_{11}, C_{22} and C_{33} are larger than C_{44}, C_{55} and C_{66}, indicating that $XFeB_4$ are mechanically anisotropic and the shear deformation is easier to take place than other deformation forms.

The elastic constant C_{66} is the most significant parameter than C_{55} and C_{44}, which implies a strong resistance to monoclinic shear in the (001) plane. The highest C_{66} for $XFeB_4$ than those for the other compounds means that its ability to resist shear distortion in the (001) plane is the strongest. The results in table indicate that $XFeB_4$ have relatively strong anisotropic elastic constants resulting in the directional dependence of the moduli. Notably, the values of C_{22} (C_{66}) are relatively higher than that of C_{11} (C_{44}) and C_{33} (C_{55})

The other compression modulis (C_{12}, C_{13} and C_{23}) are different; they correspond to the intra and inter-layer moduli under bi-axial stress conditions.

The mechanical stability criteria can be represented in a uniform manner for orthorhombic structure according to the Born stability criteria [6]

$$C_{ii} > 0 (i = 1; 2; 3; 4; 5; 6),$$

$$C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0, (C_{11} + C_{22} - 2C_{12}) > 0; (C_{11} + C_{33} - 2C_{13}) > 0,$$
$$(C_{22} + C_{33} - 2C_{23}) > 0$$

The listed results concerning $ScFeB_4$in Table-3- could not be compared because there is no study in the literature

Table-4-. Bulk B, shear G and Young modulus E (in GPa), B/G ratio, G/B ratio, Poisson's ratio ν, hardness Hv (in GPa), and Debye temperature θ_D (in k) for XFeB4 (X = Y ; Sc)

Composants	B	G	E	B/G	G/B	ν	Hv	TETA D(k)
$YFeB_4$	240	174.1	420.5	1.379	0.72	0.21	24.64	876.15
	210.73[b]	190.47[b]	439.10[b]	1.10[b]	0.90[b]	0.15[b]	35.31[b]	910[b]
$ScFeB_4$	234.84	201.26	469.62	1.167	0.85	0.17	33.01	1049.3

[b] Ref article: Abdullah Candan et al 2019 Phys. Scr. 94 125710

B/G ratio could be used to determine the brittleness or ductility of a material. If B/G ratio is higher than (1.75), the material is ductile while if it is lower than (1.75) it is brittle . All the investigated compounds are brittle because of having B/G ratio lower than (1.75) G/B ratio also called Pugh's modulus and Poisson's ratio (ν) have been calculated to determine the bonding type of the studied materials. If G/B ratio is around (1.1), this means that the material has the covalent bonding dominantly. If the material has the ionic bonding dominantly, then it has G/B ratio around 0.6 [7-23].

The bulk modulus B and shear modulus G are calculated by Voigt–Reuss–Hill approximation, which can be expressed by the following equations:

$$B = (BV+BR)/2 \quad [8]$$

$$G = (GV+GR)/2 \quad [9]$$

Young's modulus E and Poisson's ratio υ can be calculated from the following equations:

$$E = (9BG)/(3B+G) \quad [10]$$

$$\upsilon = (3B-2G)/[2(3B+G)] \quad [11]$$

A universal elastic anisotropy index (A_U) is proposed, which accounts for both the shear and bulk contributions, and is given below.

$$A_U = 5GV/GR+BV/BR-6 \geq 0$$

Poisson's ratio ν characterizes the stability of the crystal against shearing strain. For a typical metal, the value is supposed to be 0.33; for the ionic-covalent crystal, the value is situated between 0.2 and 0.3; the strong covalent crystal has even smaller Poisson's ratio, which is usually below 0.15 [7-23], the calculated Poisson's ratios of our compounds $YFeB_4$ and $ScFeB_4$ range between 0.17 and 0.22. This indicates the bond's mixture character ionic-covalent in these materials.

A larger B/G value (>1.75) for a solid indicates the ductile behavior while a smaller B/G value (<1.75) usually means brittle material. Similarly, Poisson ratio ν>0.26 corresponds usually for ductile compounds [8-23]. Our two compounds are brittle due there values (B/G <1.75).

4.7.1 Hardness

Hardness is a measure of the resistance of materials against permanent deformations. It is usually measured by traditional techniques such as in Brinell, Rockwell, Vickers, or Knoop [9] and Berkovich Nano indentation[10] (Figue-7-). Materials with high hardness are technologically important for cutting tools and wear resistant coatings. It has been recognized that the hardness of strongly covalent/ionic bonded crystals is associated directly with the bond strength[11-13].

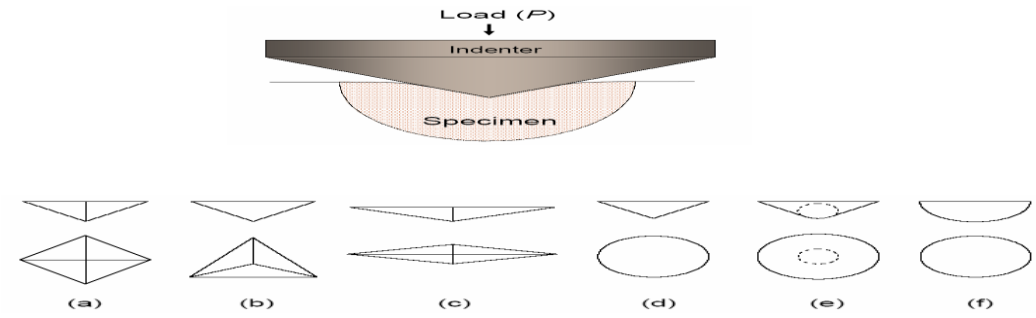


Figure -.7.- a) Hardness-resistance to penetration of a hard indenter, b) Schematics of indenter tips.

Consequently, the measured values of hardness of materials are very sensitive to many parameters including loading and unloading speed , applied load, indenter tips (Figure-7-), anisotropy of materials, defects in the sample, method of measurement, temperature, etc. Additionally, for polycrystalline materials hardness is a function of grain size; in case of thin films and coatings, their hardness depends on the repulsive barrier for the movement of dislocations across the interface between two materials and the results may vary critically (by a factor of three) with the nature of the substrate [14-17]. Therefore, it seems that there are no available methods for determining the ‘‘absolute’’ hardness of a material.

The values of our compounds $YFeB_4$ and $ScFeB_4$ are respectively; 24.6 GPa and 33 GPa, which mean that $ScFeB_4$ is harder than $YFeB_4$.

4.7.2 Debye temperture

As a fundamental parameter for the materials’ thermodynamic properties, Debye temperature ΘD is related to specific heat, thermal expansion and elastic constants. The Debye temperature can be estimated from the average sound velocity [18].

The values of our compounds $YFeB_4$ and $ScFeB_4$ are respectively; 878.2 K and 1049 K,

4.7.3 Elastic anisotropy

Most crystals exhibit elastic anisotropy of varying degree, The simplest way to illustrate the anisotropy of mechanical moduli is to plot them in the three-dimensional space as a function of direction Using equations for orthorhombic crystal system [19]:

$$\frac{1}{E} = (S_{11} + S_{22} + S_{33})l_1^4 + (2S_{12} + S_{66})l_1^2 l_2^2 + (2S_{23} + S_{44})l_2^2 l_3^2 + (2S_{13} + S_{55})l_1^2 l_3^2 \quad (21)$$

$$\frac{1}{B} = (S_{11} + S_{12} + S_{13})l_1^2 + (S_{12} + S_{22} + S_{23})l_2^2 + (S_{13} + S_{23} + S_{33})l_3^2 \quad (21)$$

In the equations above, Sij represents the compliance matrix and l_1, l_2 and l_3 are the direction cosines, which are given as $l_1=\sin\theta\cos\varphi$, $l_2=\sin\theta\sin\varphi$ and $l_3=\cos\varphi$ in the spherical coordinates.

The three-dimensional surface representations showing the variation of the Young, and bulk modulus, with The plane projections ((100), (010) and (001) plans) of the directional dependences of the Young and bulk modulus for $YFeB_4$,$ScFeB_4$ are respectevly given in (Figure-8-) and (Figure-9-)for comparisons. For an isotropic crystal, all three factors must be equal to unity, while any value deviation from1 is a measure of the degree of elastic anisotropy in the crystal.

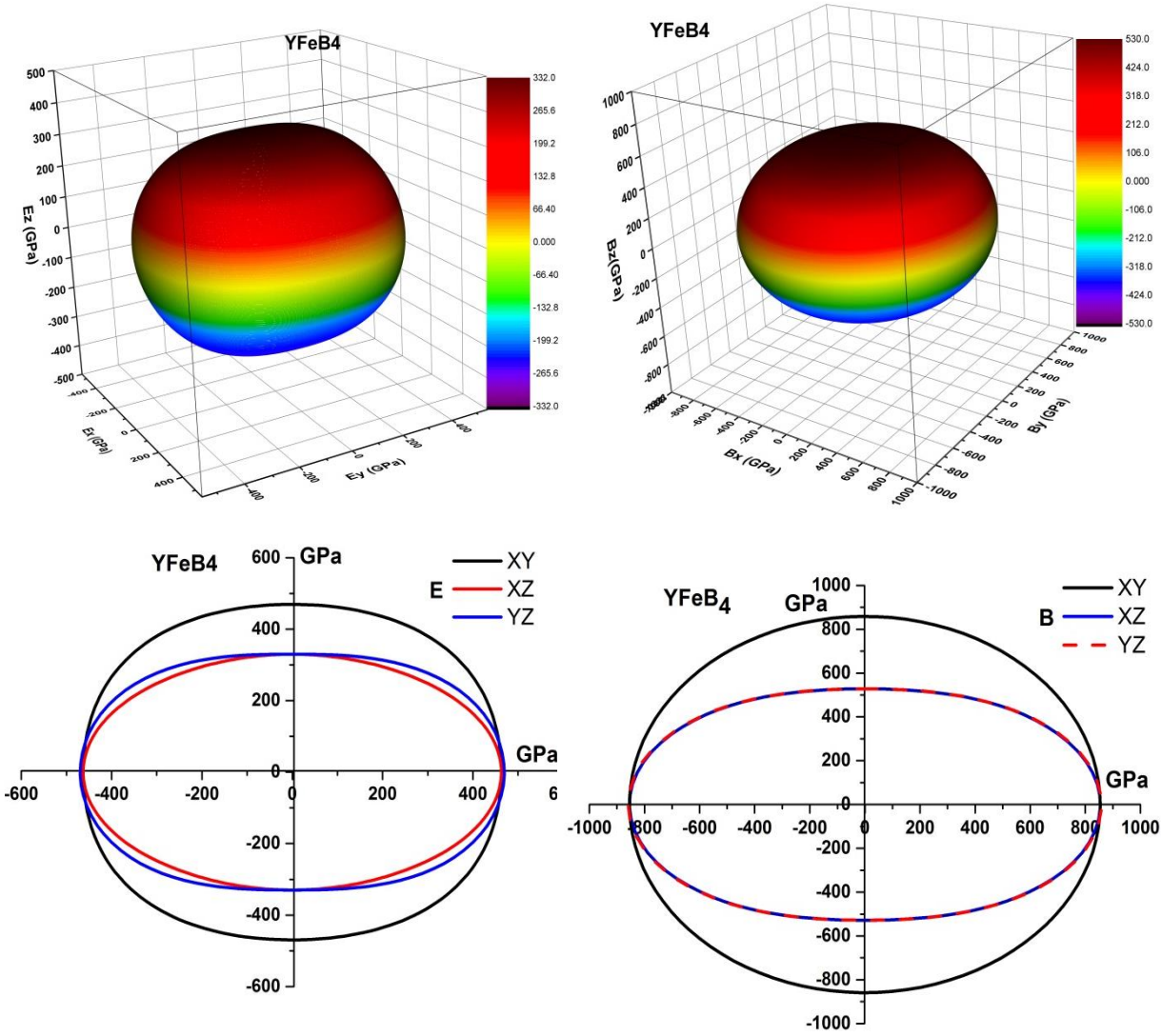


Figure-8-. Illustration of directional dependent Young and bulk modulus of $YFeB_4$ compound:

a- The Young and bulk moduli on 3D for $YFeB_4$ compounds

b- The projection of Young and bulk moduli at several different crystal planes for YFeB4 compound.

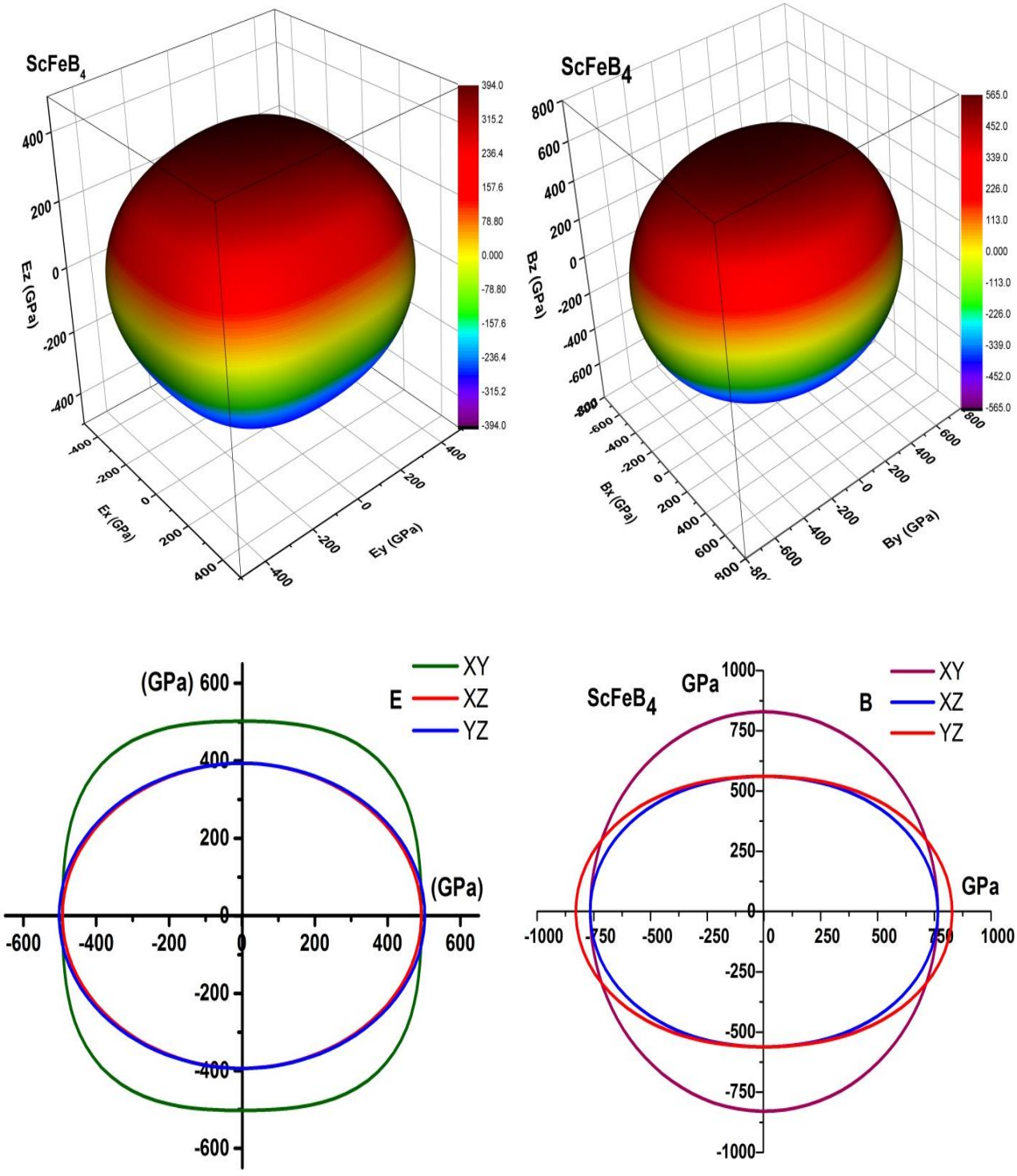


Figure-9-. Illustration of directional dependent Young and bulk modulus of $ScFeB_4$ compound:

a- The Young and bulk moduli on 3D for $ScFeB_4$ compounds

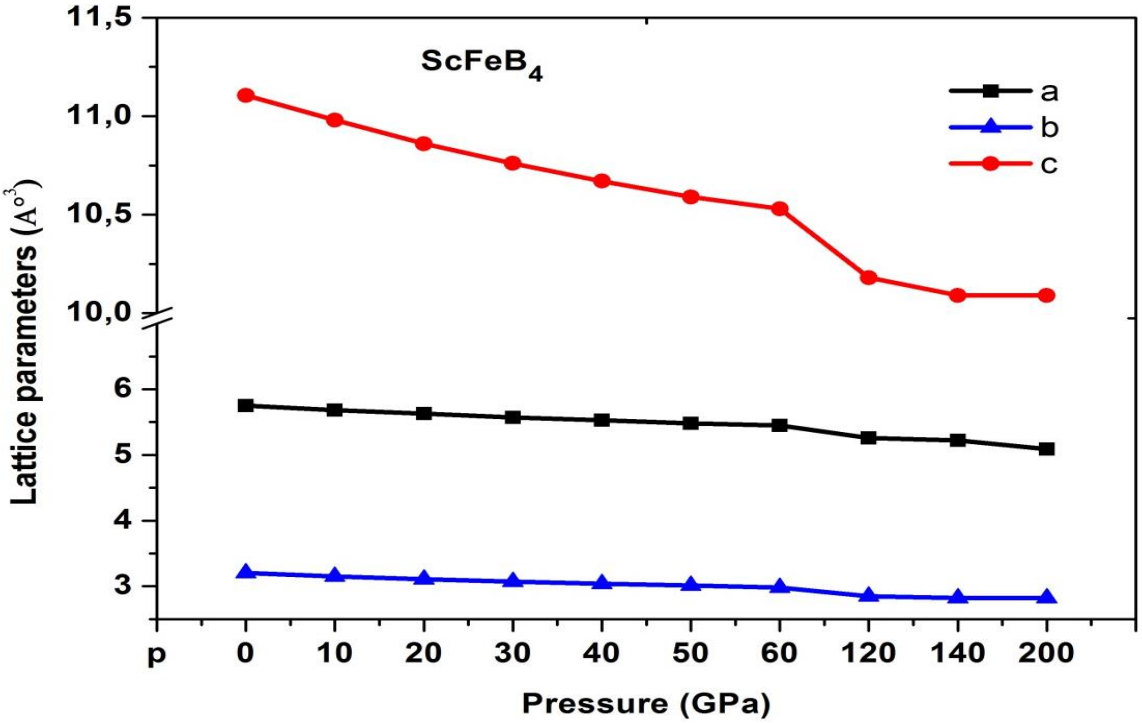
b- The projection of Young and bulk moduli at several different crystal planes for $ScFeB_4$ compound.

4.8 Structure and electronic proprieties of $ScFeB_4$ under pressure

Usually, in order to induce some significant change in the structures, high pressures are needed for the study of materials. I applied increasing pressure on my compound and examined the corresponding magnetic lattice parameters and density of state. I examined these structural properties at 0 GPa and under pressure within GGA for the $ScFeB_4$ structure, The calculated lattice parameters, unit cell volumes, are shown direction of pressure in Table -5- below

Table -5-

Pressure (GPa)	**10**	**20**	**30**	**40**	**50**	**60**	**120**	**140**	**200**
Lattice (Å)									
a					**5.750927**				
b					**11.104983**				
c					**3.204619**				
volume					**204.659635**				
a	**5.68**	**5.63**	**5.57**	**5.53**	**5.48**	**5.45**	**5.26**	**5.22**	**5.09**
b	**10.98**	**10.86**	**10.76**	**10.67**	**10.59**	**10.53**	**10.18**	**10.09**	**10.09**
c	**3.15**	**3.11**	**3.07**	**3.04**	**3.01**	**2.98**	**2.85**	**2.82**	**2.82**
volume	**196.79**	**190.09**	**184.41**	**179.42**	**174.95**	**170.96**	**153.09**	**148.59**	**148.59**



4.9 Density of state of $ScFeB_4$ under pressure

As is shown in (Figure -10-) almost the total DOS has not changed with pressure change, and the magnetic moment stayed zero. As pressure increases, the conduction band width increases because of the enhanced overlap of the wave function with the neighboring atoms

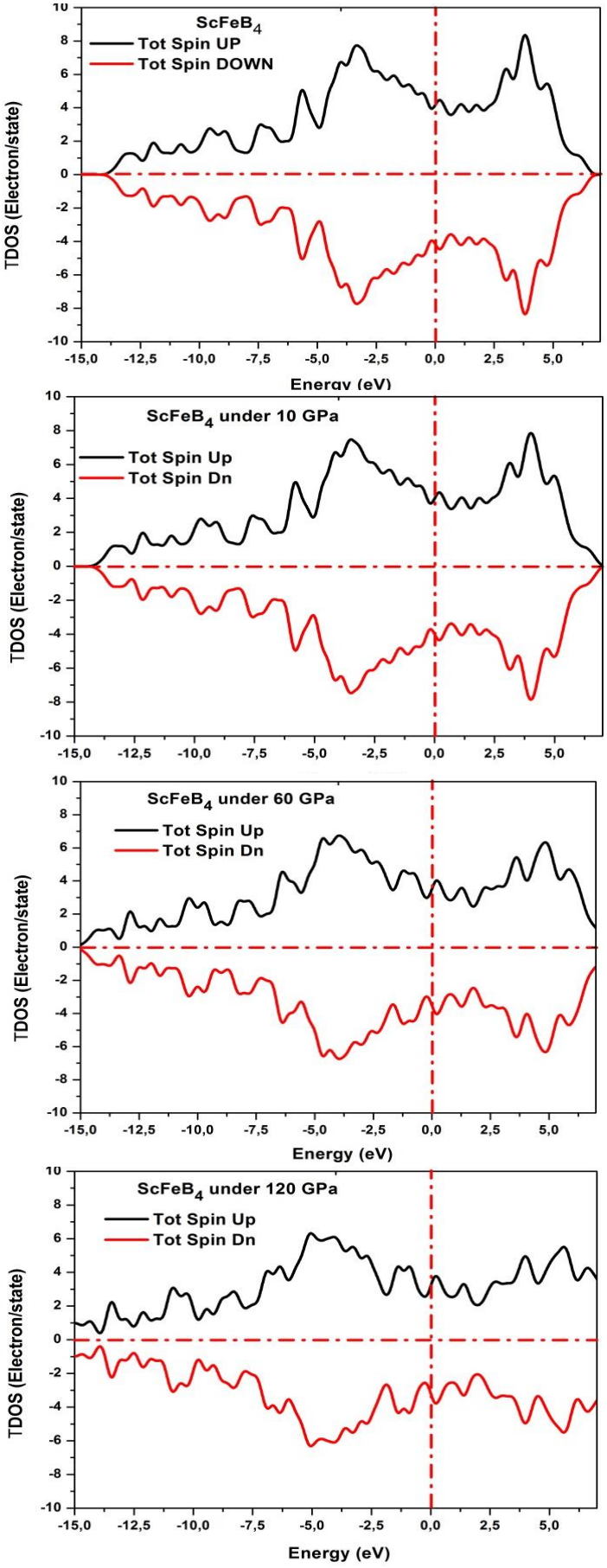


Figure-10- The calculated total DOS of ScFeB4 at 0, 10, 60 and 120 GPa. Dashed line represents the Fermi level.

4.10 Conclusion

In this thesis two compounds $YFeB_4$ and $ScFeB_4$, which they have an orthorhombic structure are investigated by density functional calculations in generalized gradient density approximation.

The first one is the $YFeB_4$ compound, where the structure and electronic properties are investigated and discussed, also, elastic moduli, hardness and elastic anisotropy properties are explored and discussed from the first-principles calculations. The calculated ground-state parameters are in good agreement with the other available theoretical data and experiments values. The strong interaction between B atoms causes an hybridization and leads to strong covalent bonds. The B/G indicate that $YFeB_4$ is brittle. The $YFeB_4$ compound show a certain degree of mechanical anisotropy

The credibility of our results cited before has encourage me to continue for another compound, which is the second compound $ScFeB_4$, The calculated ground-state parameters are calculated at 0 GPa and under pressure to look the effect of pressure on the magnetization , unfortunately, no effect, the magnetic moment stayed zero, and we are predicted all other properties: elastic constant's, hardness and elastic anisotropy.

Our perspective is to continue our calculation for other RREs materials and explorer their propertie.

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ملخص

الهدف من مذكرة الماستر 2 هذه هو الحساب الأساسي للخصائص :الهيكلية، الإلكترونية، الصلابة ومرونة التباين للمركبين:

XFeB4 (X= Y, Sc)

أجري الحساب في إطار نظرية الكثافة الدالية بإستعمال طريقة أشباه الكمونات (PP) مع تقريب التدرج المعمم (GGA) ، المثبت في البرنامج CASTEP . النتائج المتحصل عليها تمت مقارنتها مع البيانات التجريبية، وهي على إتفاق جيّد مع النتائج في الحالة الأساسية .للحصول على وصف جيّد للسلوك الميكانيكي المركبات دون /تحت تأثير الضغط، فقد قمنا بحساب الثوابت المرونية C_{ij} و من خلالها دراسة خواص تباين المرونة للمركبات المدروسة، وتحقق استقرارها الميكانيكي، واستنادا إلى تقريب فويه-روس وهيل، اكتشفنا الخصائص المرونية للمركبات المدروسة لمتعدد البلورات وحدات الوسائط الفيزيائية المرونية(، معامل القص G، الظغط B، معامل يونغ Eوبواسون υ) حيث تم رسم مخططات السطوح (3D)ومخطط المستو (2D) لمعامل الانضغاط و معامل يونغ متعددة المستويات، للكشف عن تباين الخصائص المرونية.

الكلمات المفاتيح: نظرية الكثافة الدالية، أرض نادرة، معادن انتقالية وأشباه الفلزات، الخصائص المرونية.

Résumé:

Le but de ce mémoire de master 2 est le calcul ab initio des propriétés : structurales, électroniques, dureté, et anisotropie élastique des deux composés : XFeB4 (X= Y et Sc). Le calcul a été mené dans le cadre général de la théorie de la fonctionnelle de la densité (DFT) moyennant la méthode pseudo potentiels (PP) avec l'approximation du gradient généralisé de Perdew-Burke-Ernzerhof (GGA-PBE), qui est implanter dans le code de calcul CASTEP. Les résultats obtenus ont été commentés et comparés avec les données expérimentales disponibles. Un très bon accord a été trouvé entre les résultats calculés à l'état fondamentale et ceux issus de l'expérimentale. Pour une bonne description du comportement mécanique des matériaux considérés, nous avons calculé d'abord leurs constantes élastiques en état monocristallin, i.e., les constantes élastiques anisotropes *Cij*. Les valeurs numériques obtenues pour les *Cij* ont été ensuite employées pour quantifier l'anisotropie élastique des systèmes étudiés, vérifier leurs stabilité mécanique. En utilisant toujours les valeurs des *Cij* et en se basant sur l'approximation de Voigt-Reuss-Hill, nous avons exploré les propriétés élastiques des composés étudiés en état polycristallin : les modules d'élasticité isotropes (module de compressibilité *B*, module de cisaillement *G*, module de Young *E* et rapport de poisson *υ*), Nous avons tracé les surfaces (3D) et les contours planes des modules (E et B à plusieurs plans cristallographiques, pour révéler leur anisotropie élastique.

Mots clés: DFT, Pseudo potentiels, Terre rares, métaux de transition et métalloïdes, propriétés élastiques.

Abstract:

The aim of this thesis is the ab initio calculation of the properties: structural, electronic, hardness and elastic anisotropy of two compounds: XFeB4 (X= Y and Sc). The calculation is conducted in the framework of the functional theory of density (DFT) through the pseudo potential method (PP) with the generalized gradient approximation of Perdew-

Burke Ernzerhof (GGA-PBE), which is implanted in the CASTEP code. The results are discussed and compared with experimental data. A good agreement is find between the results in the fundamental state and those from the experimental. For a comprehensive description of the mechanical behavior of the considered, I first calculate their elastic constants of single crystal state, i.e., the anisotropic elastic constants Cij. We have plotted the three-dimensional (3D) surfaces and planar contours of bulk and Young moduli of XFeB4 (X= Y and Sc). structures at several crystallographic planes, ((100), (010) and (001)) to reveal their elastic anisotropy.

Keys words: DFT, Pseudo-potential, Rare earth, transition metal and metalloid, elastic properties.