An-Najah National University
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Electronic and Structural Properties of ScSb and ScP Compounds Under High Pressure

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Dedication

To my Mother and Father

To my Sisters and Brothers

To my daughters ;Layan, Lana, Raneem

To my Sons, Mohammed, Obada

To who encouraged and supported me

My wife

Acknowledgements

I would like to express my gratitude to my supervisors, Dr. Mohammed S. Abu Ja'far and Dr. Abdel-Rahman Abu Labdeh, for their understanding, patience and valuable supervision and assistance at all levels of my graduate program. I must also acknowledge Dr. Musa El-Hasan for his continuous motivation and fruitful guidance.

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A very special thanks goes out my family for the support they provided me through my entire life and, in particular, I must acknowledge my wife and my children without whose love, patience and encouragement, I would not have finished this thesis.

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الإقرار

أنا الموقع ادناه مقدم الرسالة التي تحمل العنوان:

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Electronic and Structural Properties of ScSb and ScP Compounds Under High Pressure

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الخصائص الالكترونية والتركيبية لمركبي اسكانديوم انتمونايد وسكانديوم فوسفايد

تحت تأثير ضغط عالي

أقر بان ما اشتملت عليه هذه الرسالة إنما هي نتاج جهدي الخاص باستثناء مــا تمــت الإشارة إليه حيثما ورد وان هذه الرسالة ككل أو جزء منها لم يقدم من قبل لنيل أية درجــة أو لقب علمي أو بحثي لدى أي مؤسسة تعليمية أو بحثية أخرى.

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Declaration

The work provided in this thesis, unless otherwise referenced, is the researcher's own work, and has not been submitted elsewhere for any other degree or qualification.

Student's name:	اسم الطالب:
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Electronic and Strucural Properties Of ScSb and ScP compounds under high pressure
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Abstract

In the present study, the Full-Potential Linearized Augmented Plane Wave method that depends on the Density Functional Theory was used to investigate the structural phase transformations of ScSb and ScP compounds under high pressure.

In these calculations, the local density approximation (LDA) and the gradient generalized approximation (GGA) for the exchange correlation potential have been used . For ScSb the equations of state (EOS's) of rock-salt(RS), cesium chloride(CsCl), zincblende(ZB) and wurtzite(WZ) have been calculated, from these (EOS's), it is found that a transition under high pressure is occurred from rock salt structure to cesium chloride structure.

The transition pressure and the structural properties have also been calculated, the energy band gap for all phases of ScSb have been calculated and (-0.873,-0.683, 1.434, 1.481) eV band gaps were found and indicating that ScSb is semimetals and semiconductors respectively.

The same work was done for ScP using the same method. A number of transition phases are predicted for ScP ; rocksalt to cesium chloride and wrutzite to zincblende. The transition pressure for each case was

calculated. The structural properties have also been calculated, Finally the energy band gap for each phase was investigated.

(-0.787,-0.583, 1.578, 1.6249)eV energy band gaps are found, which means that ScP behaves as metal, semimetal and semiconductor respectively.

The most important results of this study are:

1. the structural parameters agree very well with the available experimental data and the other theoretical calculations.

2. the transition from structure to another is possible under high pressure, for ScSb the transition pressure from rocksalt to cesium chloride was found to be (31.5)GPa by LDA method and 35.4 GPa by GGA method.

3. For ScP the transition pressure from rocksalt to cesium chloride was found to be 69 GPa and from wurtzite to zincblende was found to be 84GPa by LDA method, while the transition pressure from rocksalt to cesium chloride was found to be 73.4 GPa and from wurtzite to zincblende was found to be 88 GPa by GGA method .

4. ScSb behaves as semimetal for rocksalt, metal for cesium chloride and semiconductor for zincblende and wurtzite phases using both LDA and GGA methods.

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5. ScP behaves as semimetal for rocksalt, metal for cesium chloride and semiconductor for zincblende and wurtzite phases using both LDA and GGA methods.

6. Rocksalt was found to be the ground state for ScSb and ScP compound at ambient conditions.

Chapter One
Introduction

High pressure research on structural or electronic phase transformations and behavior of materials under compression based on their calculations or measurements have become quite interesting in the recent few years; as it provides insight into the nature of the solid state theories, and determine the values of fundamental parameters[1].

The group-III-V have attracted extensive experimental and theoretical interests because of their technological applications. The question that arises; is how to extend the studies on the group III-V in order to have new class of materials with promising properties that remain too interesting in device application? One possible way is to explore new III-V compounds such as scandium antimonide (ScSb) and scandium phosphide ScP. These two compounds are semiconductors which are used in high power, high frequency applications and in laser diodes[2-6].

Recent experiments performed, by using image-plate angle dispersive X-ray techniques, for III-V group semiconductors have significantly altered the understanding of their structural systematic from the view that had been widely accepted[7]. Experimental findings as well as numerous possibilities for industrial applications initiated a number of theoretical studies of structural and electronic properties of III-V compounds[8].

Group III-V wide-gap semiconductor materials are very important because of their opto-electronic technological applications as a commercial short wavelength light-emitting diode, laser diode, transparent conductors, solar cells, high-density optical memory and visual display[9]. This importance arises from the role of the d-electrons in the valance band in hybridization, which tends to open a gap at the band crossing and make angular momentum labeling no longer suitable. The large variation of fundamental band gap (0-4eV) for these compounds yields a great flexibility for producing new III-V compounds (super-lattices and alloys) with the desirable properties to satisfy the increasing demand for such materials in various device applications as opto-electronic devices operating in the visible-light region.

Within my best knowledge, less is known about ScSb and ScP compounds. Tabboune *et al* investigated the structural and electronic properties of ScSb and ScP III-V materials within a version of the first-principles full potential linear muffin-tin orbitals method (FP-LMTO) [8]. They found that a transition from rocksalt (RS) to cesium chloride (CsCl) structure is possible at high pressure (87.75 GPa for ScSb and 330GPa for ScP). The zincblende phase (ZB) was also investigated by Tabboune *et al ;* and it was found that the ZB phase gives a semiconductor behavior with a wide bandgap.

Amrani *et al* studied the structural and electronic properties of the scandium compounds ScSb and ScP [9]. Their calculations were based on

the generalized gradient approximation (GGA) within the density functional theory (DFT), employing the first-principles full potential-linearized augmented plane wave (FP-LAPW) method. In their study, Amrani *et al* investigated the bulk properties, including lattice constants, bulk moduli and their derivatives, and band structure in both (RS) and (CsCl) structures. They found that a transition pressure from the RS to the CsCl can occur at 39.78 GPa for ScSb.

Hayashi *et al* [10] used synchrotron radiation and powder X-ray diffraction methods to study the RS structure of ScSb up to 45 GPa at room temperature. They found that a first-order phase transition from RS to CsCl structure can occur at around 28 GPa.

Recently, Xue *et al* [11] have investigated the electronic, dynamical, and thermodynamic properties of the (RS) phase for ScX (X = N, P, As, Sb) using a plane-wave pseudo potential method within the generalized gradient approximation in the frame of density functional perturbation theory [11]. They concluded that the calculated lattice constants to be differ by less than 0.56% from the available experimental values. They also concluded that these materials have wide indirect Γ–X band gaps and direct band gaps at the X-point in band structure.

In the present study, we calculate the structural and electronic properties of ScSb and ScP. Our calculations are based on the generalized gradient approximation (GGA) and local density approximation (LDA) within the density functional theory (DFT), employing the first-principles

full potential-linearized augmented plane wave (FP-LAPW) method as implemented by WIEN2K Code [12]. The wave function is expanded in atomic orbitals in spherical regions around the atomic positions; while in the region between the spheres, it is expanded in plane waves. The wave functions and their derivatives are made continuous at the boundary of the spheres, for more details see chapter two. The FP- LAPW method places no restrictions on the form of crystalline potential and is known to yield reliable structural parameters for semiconductors, metals, and insulators.

Bulk properties (including lattice constants, bulk moduli and their derivatives, transition pressure and band structure in RS, CsCl, ZB and WZ structures are investigated for both ScSb and ScP compounds.

One of the factors which stimulated me to search this subject is the lack of information about the ScP compound. Another prominent factor is the contradiction of results reached in the former studies such as lattice parameters and transition pressure.

The aim of this study, therefore, is to investigate

1- the structural parameters of the RS, CsCl, ZB and WZ phases for both ScSb and ScP,

2- the total energy for different values of lattice constant.

3- the value of transition pressure from RS phase to CsCl phase .

4- the band structure of the above phases for ScSb and ScP.

This thesis, is organized as follows:

Chapter two presents the density functional theory. Chapter three contains the method used in the calculations. Chapter four reports and discusses our results. Finally, chapter five summarizes our main conclusions .

Chapter Two
Density Functional Theory

2.1 Introduction

It is not easy in solid state to solve Schrödinger equation exactly for many- body systems, but we can obtain an approximation solution by using density functional theory (DFT). Hence the name density functional theory comes from the use of functionals of the electron density [13,14].

This theory is a theory of electronic structure that based on the electron density distribution $n(r)$ instead of many- electron wave function $\Psi(r_1, r_2, r_3, ………..)$,. so it becomes useful to understand and calculate the ground state density $n(r)$ and the energy E for any system consisting of nuclei and electrons[15].

As we know the solid is a collection of heavy nucleus and light electron particles. If we have N nuclei with each one has Z electrons so we will deal with N+ZN electromagnetically interaction particles that is called many- body interactions problems, then we need quantum many body problem to study these materials and their properties. This means that we must solve the independent Schrödinger equation:

$$\hat{H}\, \Psi = E\, \Psi \qquad\qquad (2.1)$$

where Ψ is the wave function for all participating particles and $\hat{H}$ is the many-particle Hamiltonian which is given by :

$$\hat{H} = T_n + T_e + V_{ee} + V_{en} + V_{nn} \qquad\qquad (2.2)$$

where T_n is the kinetic energy operator for the nuclei, T_e is the kinetic energy operator for the electons, V_{ee} is the potential energy due to the interaction between the electrons, V_{en} is the potential energy due to the electrons nuclei interaction and V_{nn} is the potential energy due to the nuclei –nuclei interaction.

It is difficult to solve this problem exactly, so we must find acceptable approximation solution .

2.2 The Born-Oppenheimer Approximations

Because the nuclei are heavier and slower than the electrons, Born-Oppenheimer assume that the nuclei do not move any more, and hence their kinetic energy are neglect (equal to zero). So the first term of equation 2-2 disappears and the last term reduces to be constant. So we are left with the kinetic energy of the electrons and potential energy due to electron-electron interactions and due to electrons- nuclei interactions. Hence equation 2-2 becomes

$$\hat{H} = T_e + V_{ee} + V_{en} + \text{constant} \qquad (2.3)$$

Equation 2-3 can be written as :

$$\hat{H} = T_e + V + V_{ext} \qquad (2.4)$$

where T_e the electron kinetic energy, V the potential due to electron-electron interactions and V_{ext} the potential energy of the electrons in the (now external) potential of the nuclei[16].

2-3 Density Functional Theory (DFT)

DFT is a variational theory in which the total energy of a system can be written in terms of the charge density only . In this scheme, the exchange – correlation energy is written as a local function of the density. The variational problem is then explained by solving the Kohn-Sham (KS) equations using self-consistently method [17,18].

Density Functional Theory (DFT) is an exact theory for a ground state of a quantum many-body system, and it states that the ground state properties depend exclusively on the ground state electronic density, and not on the full details of the wave function[19].

2-3.1 Hohenberg and Kohn Theorem

Hohenberg and Kohn have shown that the ground state electron density $n(r)$ uniquely, defines the total energy E, (i.e., $E=E(n)$)

Also they have shown that the ground state density is the density that minimizes $E(n)$because the the ground state properties are functionals of the ground state density[20].

2-3.2 Kohn Sham (KS)Equations

KS equations are similar in form to the time-independent Schr dinger equation, expect that the potential experienced by the electrons is formally expressed as a functional of the electron density[21].

In the KS method the density is given by the solutions of a one electron Schr dinger equation for a periodic potential formed varationally from the total energy expression[22]. Kohn and Sham introduced a method that enables one to minimize the functional *E(n(r))* by varying *n(r)* over all densities containing N electrons.

Kohn and Sham devided *E(n(r))* into four parts . So the energy *E(n(r))* becomes

$$E(n(\vec{r})) = T_s(n(\vec{r})) + \frac{1}{2}\iint \frac{n(\vec{r})n(r')}{|\vec{r}-r'|}d^3rd^3r' + E_{XC}(n(\vec{r})) + \int n(\vec{r})V_{ext}(\vec{r}))dr \quad (2.5)$$

Where the kinetic energy $T_s(n(\vec{r}))$ of a non-interacting electrons is given by:

$$T_s(n(\vec{r})) = -\frac{1}{2}\sum_{i=1}^{N}\int \psi_i^*(\vec{r})\nabla^2\psi_i(\vec{r})dr \quad (2.6)$$

In terms of an effective potential, $V_{eff}(r)$, we can rewrite Lagrange equation as :

$$\frac{\delta T_s[n(\vec{r})]}{\delta n(\vec{r})} + V_{eff}(\vec{r}) = \mu \quad (2.7)$$

where:

$$V_{eff}(\vec{r}) = V_{ext}(\vec{r}) + \int \frac{n(r')}{|\vec{r}-r'|}dr' + V_{xc}(\vec{r}) \quad (2.8)$$

and

$$V_{XC}(r) = \frac{\delta E_{XC}[n(\vec{r})]}{\delta n(\vec{r})} \quad (2.9)$$

Now, if one considers a system that really contained non-interacting electrons moving in an external potential equal to $V_{eff}(r)$, as defined previously, then the same analysis would lead to exactly the same result. To find the ground state energy and density,(E_0 and n(r)) we, therefore, need to solve the one-electron equations :

$$\left(-\frac{1}{2}\nabla^2_i + V_{eff}(\overrightarrow{r}) - \varepsilon_i\right)\psi_i(\overrightarrow{r}) = 0 \qquad (2.10)$$

As the density is constructed according to

$$n(\overrightarrow{r}) = \sum_{i=1}^{N}\left|\psi_i(\overrightarrow{r})\right|^2 \qquad (2.11)$$

The above derivation assumes that the exchange-correlation functional is known. At present numerical method, exchange –correlation potentials have only been determined for a few simple model systems[23].

2-3.3 The Local Density Approximation (LDA)

In solving Kohn- Sham equations, there is one term that we cannot find it exactly, it is the exchange-correlation energy. Thus LDA method is one of several methods that can calculated it. LDA works where the charge density is varying and depends on the local density in limited volume [24,25,26].

2-3.4 The Generalized Gradient Approximations (GGA)

In this approximation, the exchange-correlation energy is dependent on the local densities (neighboring volumes) and their gradients. So it is

improvement to LDA. Also, GGA approximation give accurate and larger equilibrium lattice parameters comparing to LDA approximation [24,25,26].

2-4 Full Potential Linearized Augmented Plane Wave (FP-LAPW) Method

It is a method used to simulate the electronic properties of materials on the basis of density functional theory (DFT). This method has been successfully applied to study structural phases transitions of certain semiconductors, which increases the number of plane waves in the basis set, in order to decrease the structural properties of systems accurately [27].

The shape of the charge density, is taken into account with high accuracy. The FP-LAPW method is an all-electron algorithm which is universally applicable to all atoms of the periodic table, in particular to transition metals, rare-earths metals and multi-atomic systems [28]. In this method, the unit cell is divided into two regions as shown in Figure 2-1:
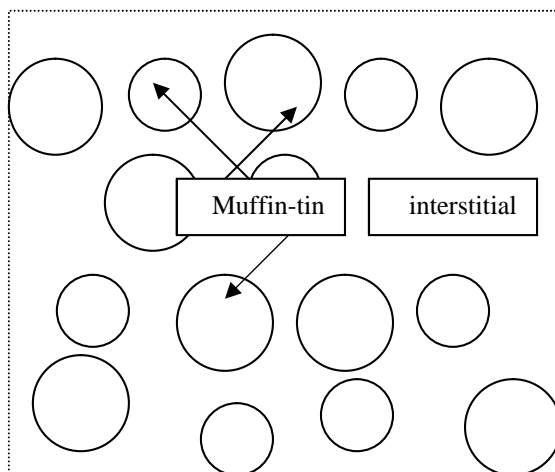

Figure (2.1): The unit cell divided into muffin-tin region and interstitial region.

1. Muffin- tin region: that occupied by muffin- tin sphere

2.Interstitial region: the space outside spheres.

The potential approximated to be spherically inside the muffin-tins, while in the interstitial region the potential is set to be constant. Therefore, the plane wave solve the Schrodinger equation in interstitial region, and the product of radial solution times the spherical harmonic solution solve the Schrodinger equation in the muffin-tin region [29].

2.5 WIEN2K Code

The electronic structure calculations for solids can be allowed by this code using density functional theory (DFT).WIEN2k is one of the most popular electronic structure codes used to perform calculations with the FPLAPW method. Also, it is one among the most accurate schemes for band structure calculations [30].

2.6 Applications of WIEN2K Systems

2.6.1 Band Structure and Density of Sstates

Energy bands consisting of a large number of closely spaced energy levels exist in crystalline materials. The bands can be consider as the collection of the individual energy levels of electrons surrounding each atom.

The electron band gap energy of a solid describes ranges of energy that an electron is forbidden to have. It is due to the diffraction of the

quantum mechanical electron waves in the periodic crystal lattice. The band structure of a material determines several characteristics such as understanding the concept of an energy band gap [31].

The density of states (DOS) of a system describes the number of states at each energy level that are available to be occupied. A high DOS at a specific energy level means that there are many states available for occupation. The energy band structure and the corresponding density of states are the dominant quantities that determine the electronic structure of a system. Hence, their inspection provides information about the electric property, (metal, insulator or semiconductors) [32].

2.6.2 Electron Densities

Electron density is the measure of the probability of an electron being present at a specific location. Regions of electron density are usually found around the atom, and its bonds. The electron density is the key quantity in DFT as mentioned before[20].

2.6.3 Total Energy and Phase Transitions

The relative stability of different phases can be computed by the total energy. In such cases it is possible to keep many parameters constant as possible in order to have a cancellation of systematic errors[33]. These parameters for example, the atomic size of spheres, the plane-wave cut-off, the k-mesh, the DFT functional the treatment of relativity, etc. Because the

energy differences are small, so a consistent treatment of the systems to be compared will help to minimize these computational effects [34].

2.6.4 Equilibrium Volume and Bulk Modulus

The total energy calculations as a function of volume can be done by fitting to an equation of states according to Murnaghan's equation[35]:

$$E(V) = \frac{B_0 V}{B_0^{/}} \left[\frac{\left(\frac{V_0}{V}\right)^{B_0^{/}}}{B_0^{/}} + 1 \right] + C \qquad (2.12)$$

where V_0 is equilibrium volume, B_0 and $B_0^{`}$ are the bulk modulus and its derivative.The equilibrium volume and the bulk modulus can be calculated from the above equation by plotting the total energy versus volume.

Chapter Three
Crystal Structures and Computational Details

3-1 Introduction

The crystal is a solid that composed of basis (atoms or microscopic particles) arranged in an periodic array. This arrangement of the basis is called crystal structure. Hence, we can define the crystal structure as lattice plus basis.

The crystal structure of a material can be described in terms of its unit cell. Some of unit cells known as primitive cells because each of primitive cell contains one lattice point. [36].

There are seven of Bravais lattice which are distinguished from one to another by the angles between the three axis, but we are dealing with two types in our study (cubic and simple hexagonal).

In the case of cubic lattice, the lattice parameters of its unit cell are: a = b = c . Also, the lattice axes are perpendicular to one another α = β = γ = 90 The cubic lattice may be simple, body – centered or face centered.

The primitive unit vectors for simple cubic can be taken as:

$$\vec{a_1} = a\hat{x} \qquad \vec{a_2} = a\hat{y} \qquad \vec{a_3} = a\hat{z}$$

Also, the primitive unit vectors for face centered cubic can be taken as:

$$\hat{a}_1 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z} \qquad \hat{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z} \qquad \hat{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$

The primitive unit vectors for body – centered cubic can be taken as:

$$\vec{a_1} = \frac{a}{2}(-\hat{X} + \hat{y} + \hat{z})$$

$$\vec{a_2} = \frac{a}{2}(\hat{X} - \hat{y} + \hat{z})$$

$$\vec{a_3} = \frac{a}{2}(\hat{X} + \hat{y} - \hat{z})$$

In the case of hexagonal lattice, however, the lattice parameters of the unit cell are: $a = b \neq c$. Also the angle between a and b axes is $60°$, while the third is perpendicular to both of them [32, 33].

The primitive unit vectors for simple hexagonal can be taken as:

$$\vec{a_1} = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y} \qquad \vec{a_2} = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y} \qquad \vec{a_3} = c\hat{z}$$

3-2.Crystal structures

3-2.1 Rocksalt Structure (RS)
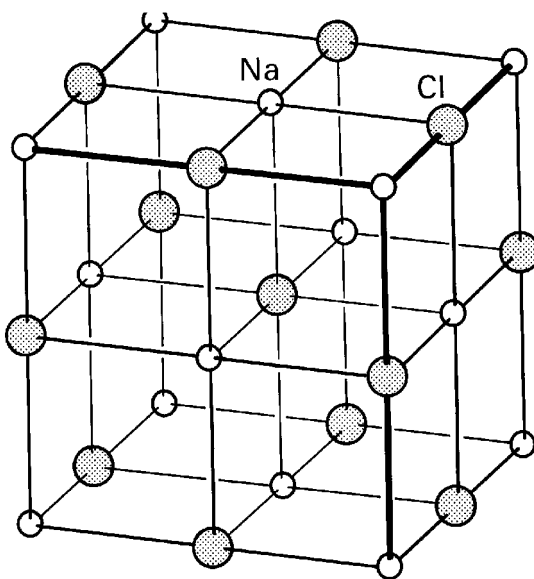
The rocksalt structure is shown in Figure 3.1

Figure (3.1): Rocksalt Structure

Rocksalt has face centre cubic lattice with two basis :Na at position (0, 0, 0)a and Cl at position (0.5, 0.5, 0.5)a where a is the lattice parameter[32,33,37].

3-2.2 Cesium Chloride Structure (CsCl)

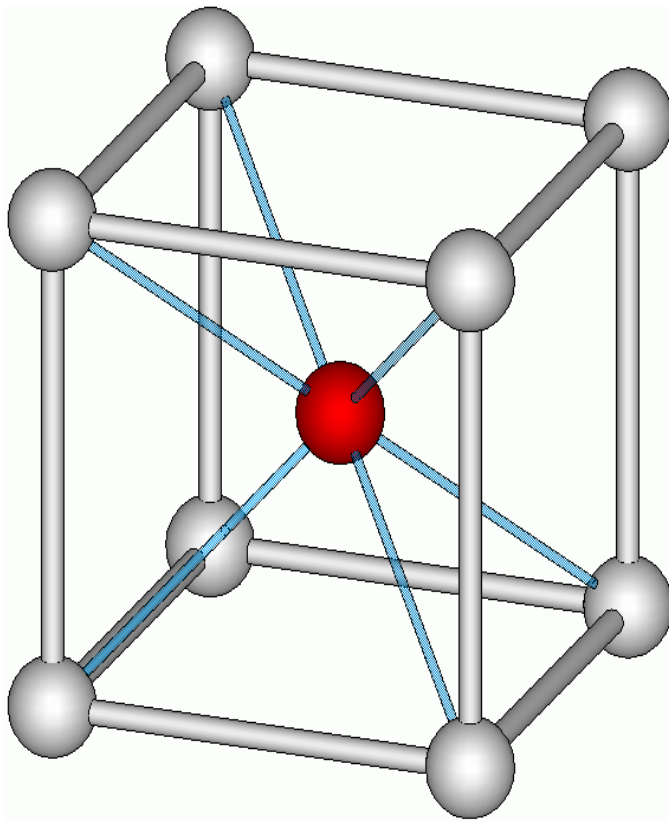The cesium chloride structure is shown in Figure 3-2,

Figure (3.2): Cesium Chloride Structure

Cesium chloride has simple cubic lattice with two basis :Cs at position (0,0,0)a and Cl at position (0.5,0.5,0.5)a[32,33,37] .

3-2.3 Zincblende Structure (ZB)
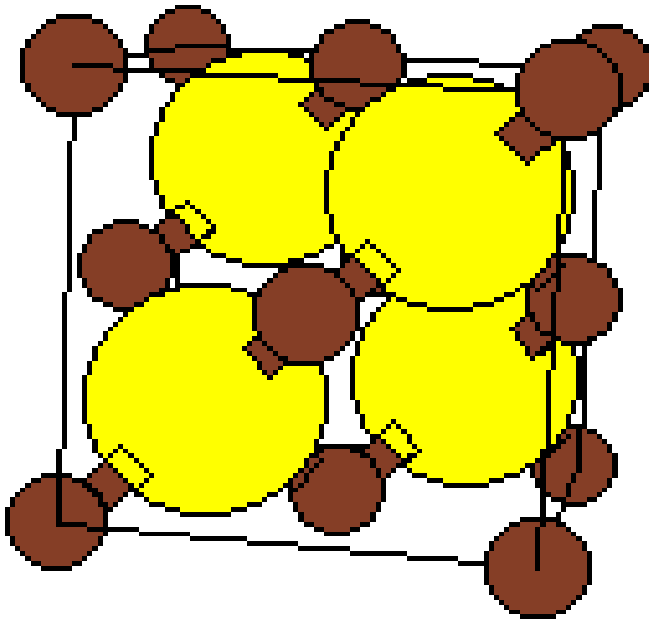
The zincblende structure is shown in Figure (3-3),

Figure (3.3) :Zincblende Structure

Zincblende structure has face centre cubic lattice with two basis :Zn position at (0,0,0)a and S at position (0.25,0.25,0.25)a [32,33,37].

The difference between the RS structure and ZB structure due to how the two lattices are positioned relative to one another[38].

3-2.4 Wurtzite Structure (WZ)

The wurtzite structure is shown in Figure 3.4.
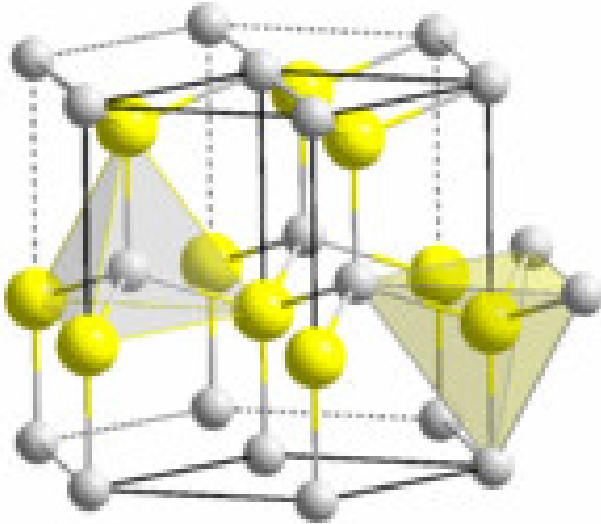
Figure (3-4): Wurtzite structure

Wurtzite has simple hexagonal lattice with two basis. The position of the first basis is at (1/3,2/3,0)a and the second is at (1/3,2/3,u)a where u=3/8 with c/a=(8/3)$^{1/2}$[32,33,37].

3-3 Computational Details

In this study the structural phase transition of ScP and ScSb have been investigated under high pressure with full-potential linear augmented wave (FP-LAPW) implemented by WIEN2K computer code within the local density approximation (LDA) and generalized gradient approximation (GGA).

In the present study, the FP-LAPW results for the crystal charge density were obtained with LDA (which proposed by Perdew and Wang) and GGA

which proposed by Perdew and his co-workers[39]. The FP-LAPW method is used to calculate the electronic structure and the total energy of ScP and ScSb in the CsCl, WZ, ZB and rocksalt phases. The FP-LAPW program,WIEN2K, is used to solve the Kohn-Sham equations. In FP-LAPW method, the wave function is expanded in atomic orbitals in spherical regions around the atomic positions, while in the regions between the spheres, it is expanded in plane wave. The wave functions and their derivatives are made continuous at the boundary of the sphere. The FP-LAPW places no restrictions on the form of crystalline potential and is known to yield reliable structural parameter for semiconductors, metals and insulators[40]. Spin-orbit effects are not included in the calculations.

Plane cut-off is chosen from the condition Rmt Kmax = 8 for LDA and Rmt Kmax =9 for GGA calculations, where Kmax is the plane wave cut-off and Rmt is the atomic sphere radius (muffin-tin radius). A sufficiently dense k-point grid was used to achieve a good and very close convergence of total energy. We have used k-point= 3000 with reduced k=104 and matrix = 14x14x14 for ScSb in the RS, CsCl and ZB structures. While we have used k-point=1000 with reduced k=76 and matrix 12x12x6 for WZ structure. We have used k-point = 3000 with reduced k = 84 and matrix of 14x14x14 for ScP in the CsCl, ZB and RS structures; while we used k-point=1000 with reduced k=76 and matrix 12x12x6 for WZ structure.

The calculated bulk properties are obtained by fitting the calculated total energy to the Murnghan's equation of state. In order to keep the same

degree of convergence for all the lattice constants studied, we kept the values of the sphere radii constant over all the range of lattice spacing considered. For ScSb compound we have considered Rmt to be 2.5 A^0 for both Sc and Sb atoms. For ScP, we have also considered Rmt to be 2.5 A^0 for both Sc and P atoms. The lattice harmonics (angular momenta) up to l=10 are used for the expansion inside the muffin-tin spheres for the development of the wave function of the charge density and potential.

The ground state properties are obtained by minimization of the total energy with respect to the volume of the unit cell . In ZB, CsCl and RS structures, the volume is directly related to the lattice constant a. While for the wurtzite structure, this minimization are performed using three independent parameters, lattice constants a, c and the internal cell parameter u. Equilibrium values are found by calculating the total energies for a set of values of the c/a ratio and the volume per unit cell, to determine the optimum value of u.

The equilibrium value and bulk modulus are determined by calculating the total energies for a set of volumes and fitting these to the Murnaghan's equation of state [41]. We have calculated the total energy for 14 different values of c/a and find the location of the minimum energy by fitting the resulting values to a parabola . Freezing a and c/ a at the best values just found, we vary the parameter u and find the new minimum of the total energy . Finally, with c/a and u fixed at their optimized values, we vary a and calculate the total energy for 14 different volumes, which we fit again by Murnaghan's equation of state.

Chapter Four
Results and Discussions

4.1. Introduction

Scandium III-V based materials have recently received more attention, as mentioned before, less is known about ScSb and ScP, recent synchrotron X-ray diffraction and experimental studies have proved that ScSb can have a phase transition from the rocksalt (RS) structure to the CsCl structure, and this is also true for ScP[7].

4.2 ScSb compound

The main aim of studying this compound is to investigate the stability of its rocksalt structure . We also studied its cesium chloride, zincblende and wurtzite structures; and the transition pressure from rock salt to cesium chloride structure . We also calculated its structural parameter . Finally, we calculated its energy band gap for each phase by using the FP-LAPW method depending on the density functional theory.

4.2.1 Optimization

Most of the complicated structures have free internal structural parameters which can either be taken from experiment or optimized using the calculated forces on the nuclei. There are some suggestions about how to optimize a structure in WIEN2K:

a. start calculations by generating struct-file with arbitrary parameters, (i.e lattice parameters, positions of basis)

b. initialize your file by introducing R_{MT} K_{max},G_{max} and number of k-points.

c. Run lapw and self- consistency cycle (SCF) cycle.

d. Choose optimize (equilibrium volume V, the ratio of the height of the unit cell to its edge, c/a) job then x-optimize and choose vary transition phases.

This procedure is suitable for the four structures (rocksalt, cesium chloride, zincblende and wurtzite structures), but for wurtzite structure we found the ratio c/a by taking seven values (-6,-4,-2,0,2,4,6%), for each value writing down, a,c,c/a and run SCF to find minimum energy as shown in tables (4.1,4.2) fittng these data to a Fortran program called polyfit and then getting the best value for c/a. This was done for LDA (c/a=1.587) and GGA (c/a=1.489)

Table (4.1): Calculating c/a by LDA method

no	percent	a =b (a.u)	c (a.u)	c/a	E (RY)
1	-6	9.06681	12.96553	1.429999	-28991.60504
2	-4	9.00340	13.14879	1.460424	-28991.611612
3	-2	8.94173	13.33079	1.490851	-28991.616282
4	0	8.88172	13.51155	1.521276	-28991.619276
5	2	8.82328	13.69111	1.551702	-28991.620800
6	4	8.76636	13.86950	1.582127	-28991.621007
7	6	8.71087	14.04674	1.612553	-28991.620091

Table (4.2): Calculating c/a by GGA method

no	percent	a =b (a.u)	c (a.u)	c/a	E (Ry)
1	-6	8.70041	12.95805	1.489360	-28962.850715
2	-4	8.76168	13.04931	1.489361	-28962.855193
3	-2	8.82211	13.13931	1.4893614	-28962.858236
4	0	8.88172	13.22809	1.4893613	-28962.859837
5	2	8.94054	13.31569	1.4893610	-28962.860234
6	4	8.99859	13.40216	1.489362	-28962.859510
7	6	9.05591	13.48753	1.4893622	-28962.857791

Then we found the internal parameter u which controls the position of the atom in the unit cell by taking different values of u by running SCF calculations and then writing down the total energy for each value as shown in tables (4.3and 4.4).This was found for LDA (0.374) and for GGA (0.375)

Table (4.3): Calculating u by LDA method

no	u	E (Ry)
1	0.360	-28991.299562
2	0.365	-28991.299685
3	0.368	-28991.299701
4	0.369	-28991.299716
5	0.370	-28991.299727
6	0.372	-28991.299901
7	**0.374**	**-28991.311664**
8	0.376	-28991.299978

Table (4.4):Calculating u by GGA method

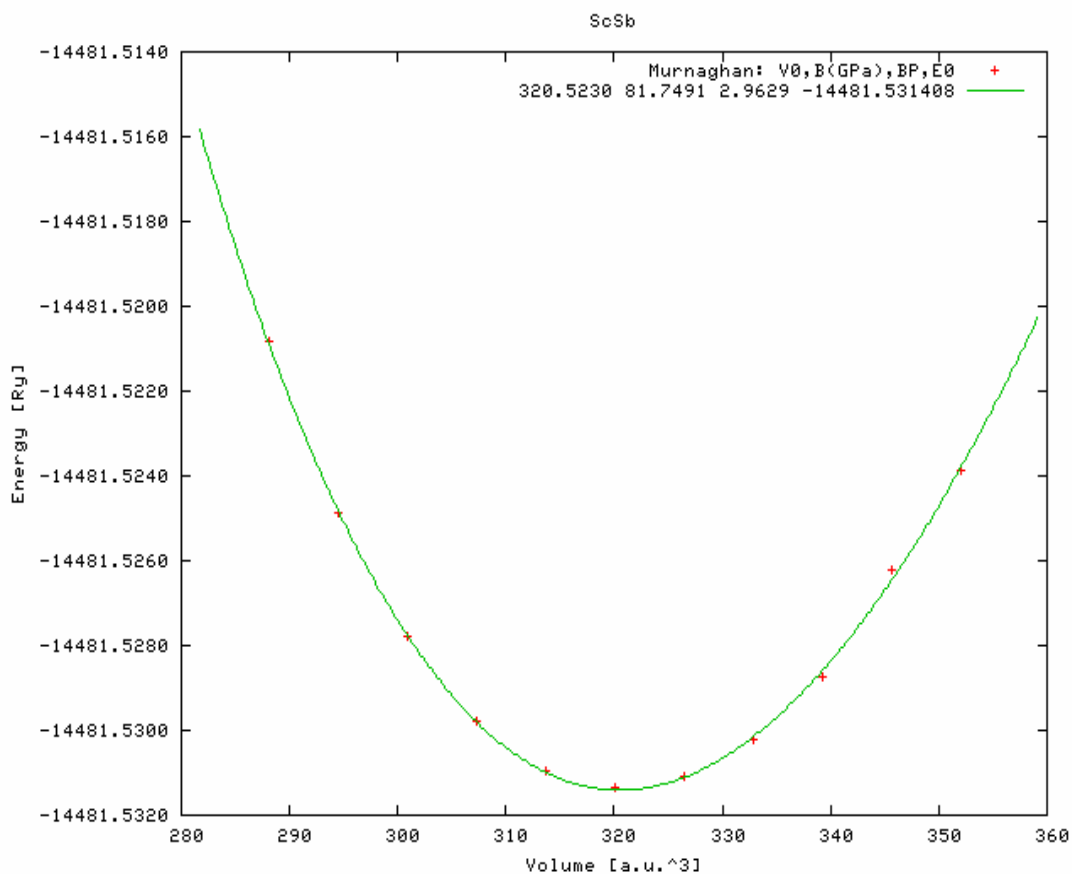| no	u	E (Ry)
1	0.360	-28962.63215
2	0.365	-28962.63278
3	0.368	-28962.63297
4	0.369	-28962.63318
5	.0370	-28962.63381
6	0.372	-28962.63401
7	0.374	-28962.63492
8	**0.375**	**-28962.63521**
9	0.377	-28962.63501

Fig (4.1a): Energy vs volume for ScSb in rocksalt structure by LDA method
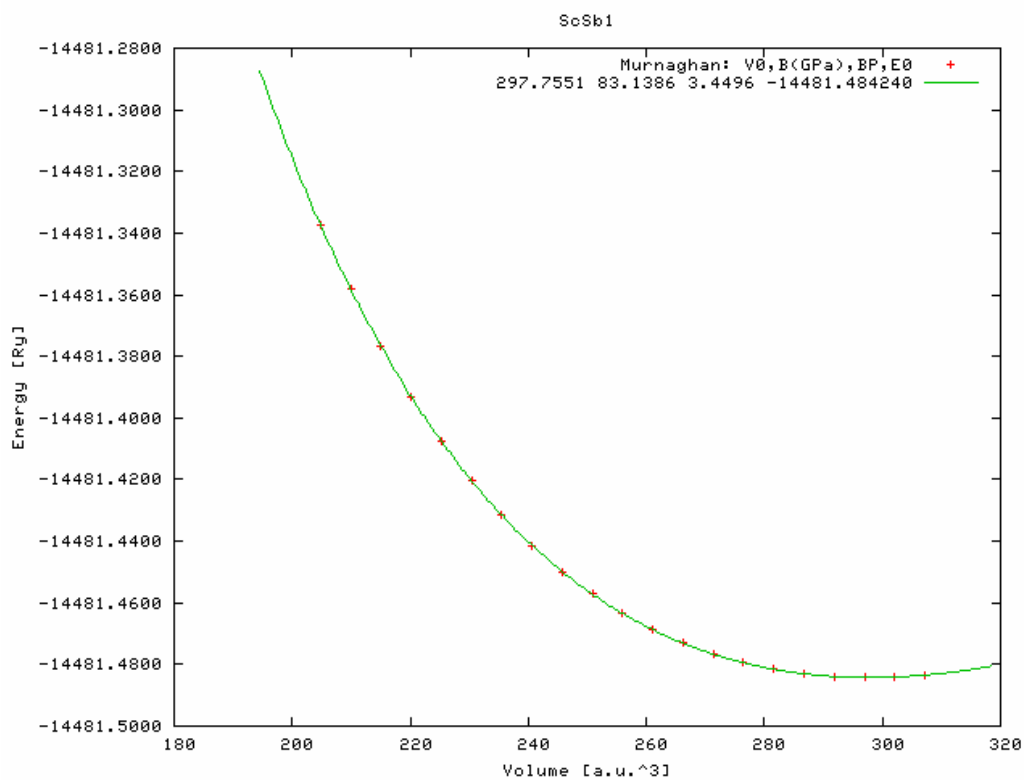

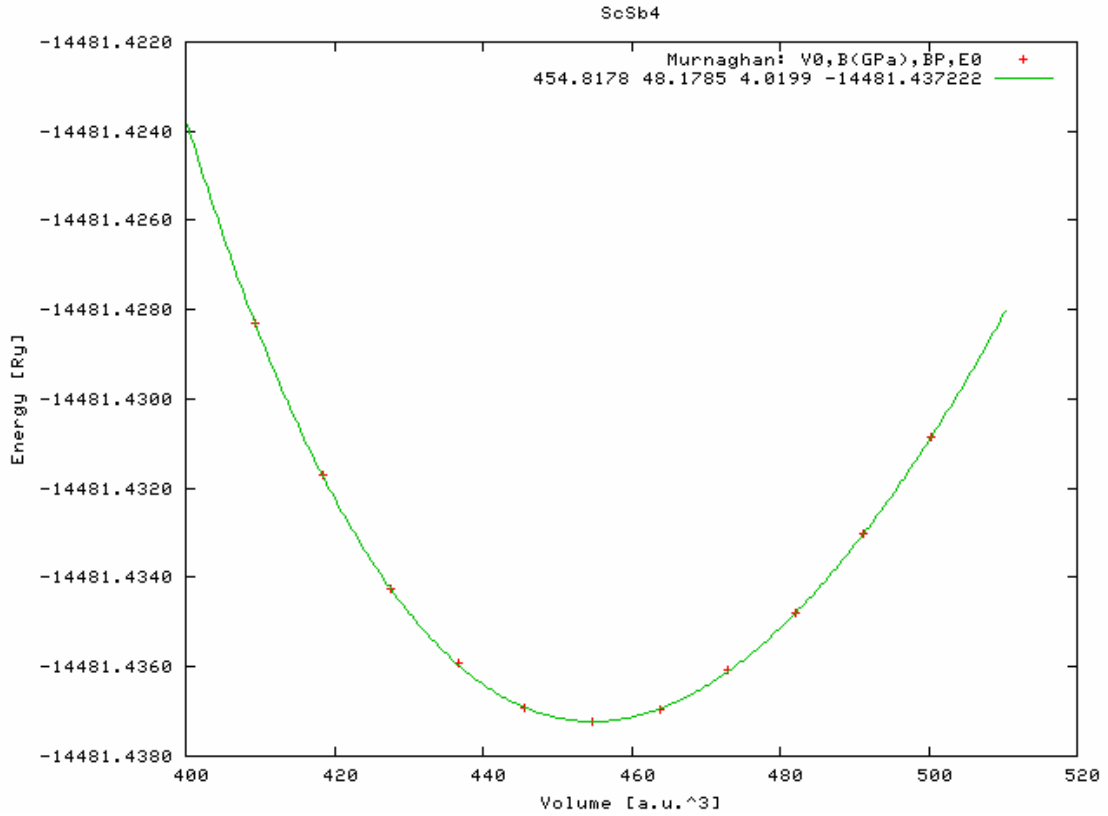**Fig (4.1 b): Energy vs volume for ScSb in cesium chloride structure by LDA method**

Fig (4.1c): Energy vs volume for ScSb in zincblende structure by LDA method
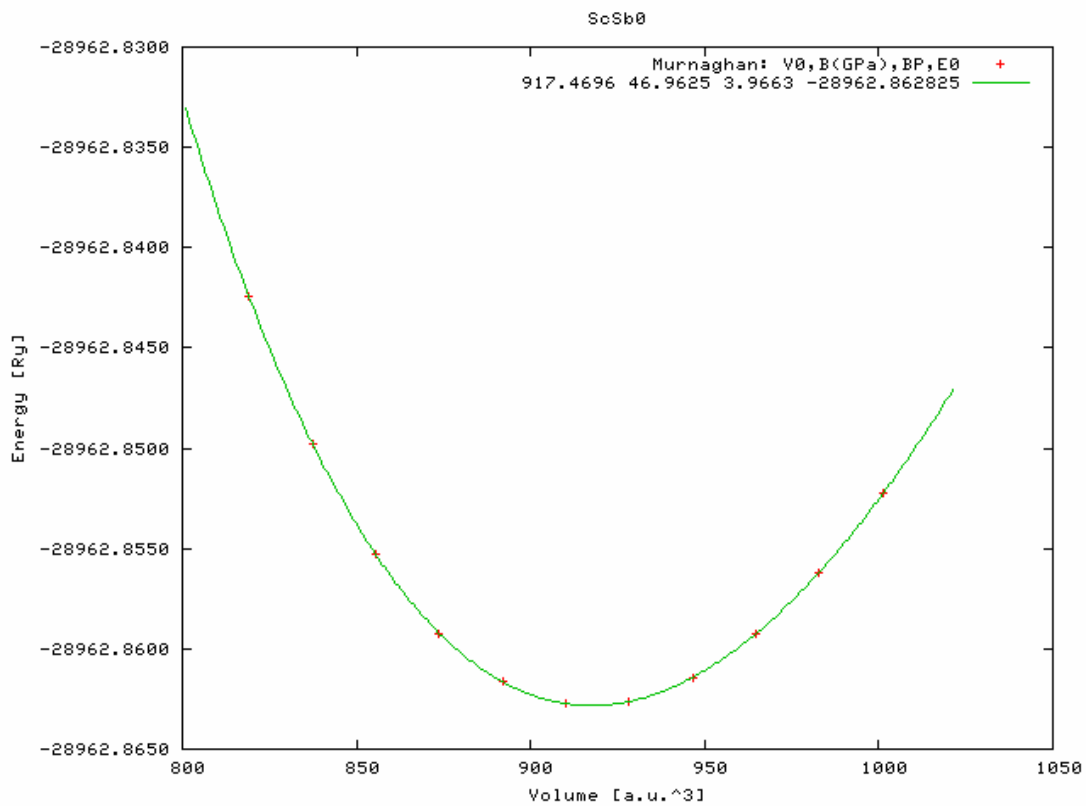

Fig (4.1d): Energy vs volume for ScSb in wurtzite structure by LDA method

Then, we use GGA approximation method to plot the energy versus volume for the fourth structures (rocksalt, cesium chloride, zincblende and wurtzite), that shown in Figure 4.2.The results are (volume, lattice parameters) summarized in table 4.5.
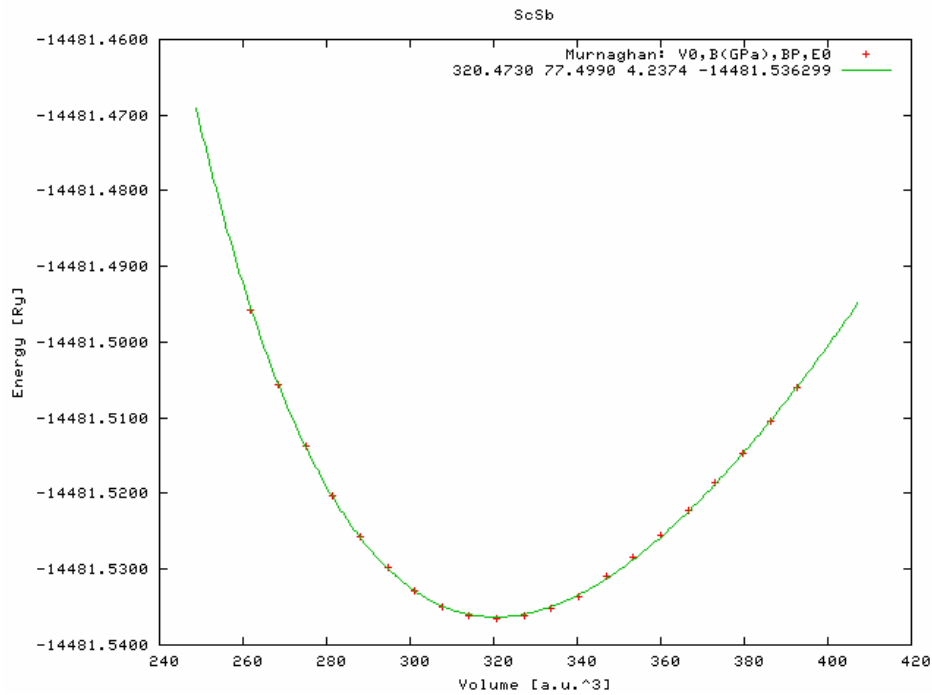

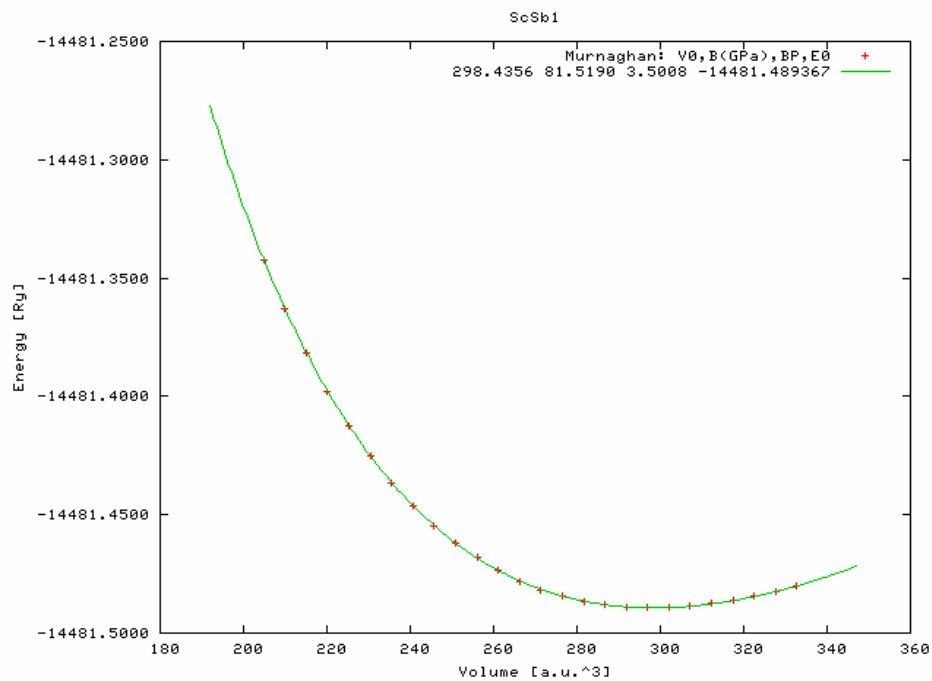**Fig (4.2a): Energy vs volume for ScSb in rocksalt structure by GGA method**

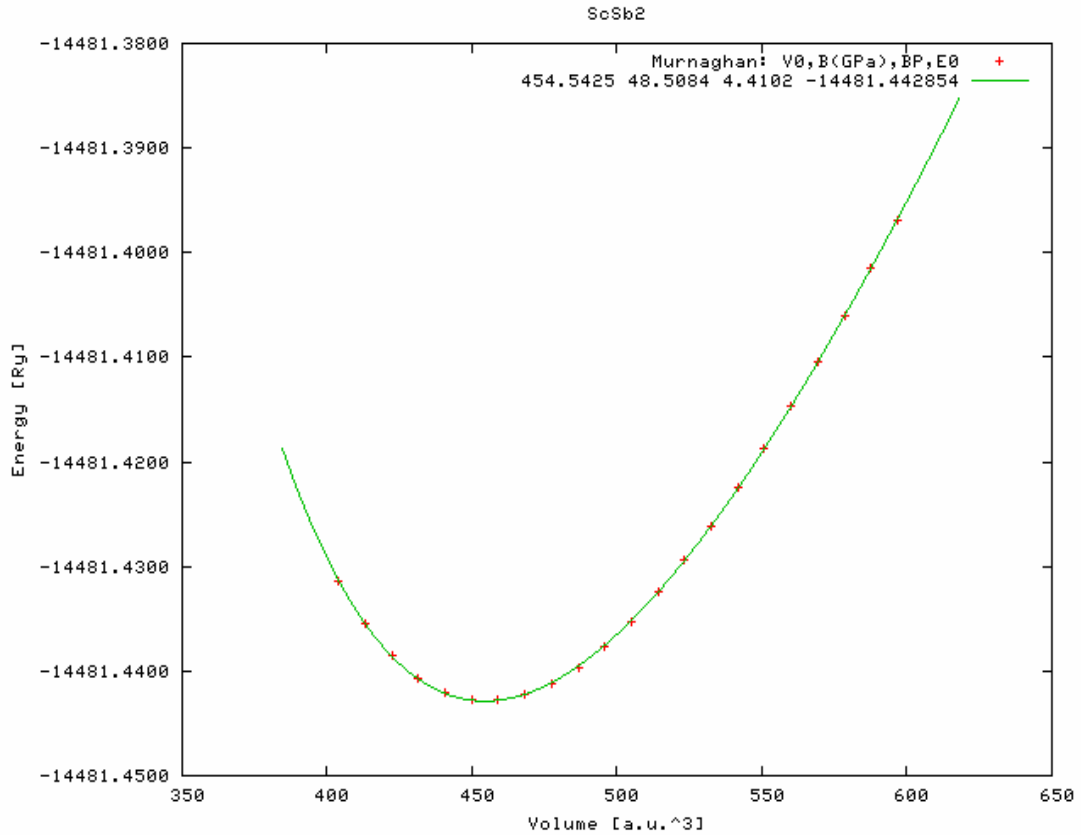**Fig (4.2b): Energy vs volume for ScSb in cesium chloride structure by GGA method**

Fig (4.2c): Energy vs volume for ScSb in zincblende structure by GGA method
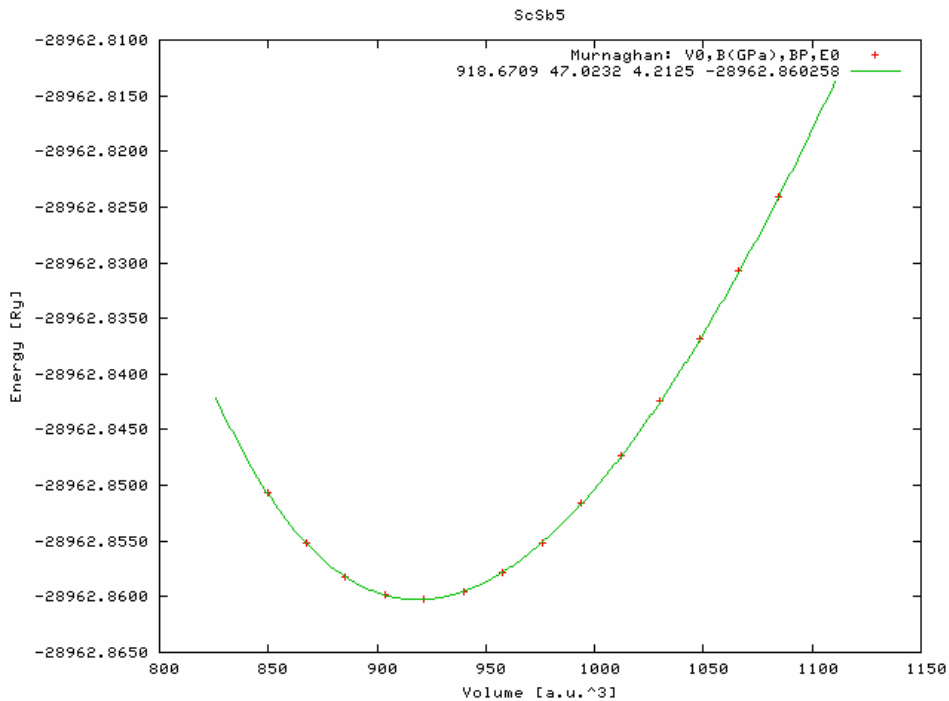

Fig (4.2d): Energy vs volume for ScSb in wurtzite structure by GGA

We found the lattice parameter a of ScSb in the four phases as shown in fig (4.1,4.2), we summarized the results in table (4.5)

Table (4.5): Structural parameters of ScSb in the four phases(RS, CsCl, ZB,WZ whereV$_0$ is the equilibrium volume, a is the lattice constant,B_0 is the bulk modulus and $B_0^`$ is its pressure derivative)

Compound	Paremeters	Rocksalt	CsCl	Zincblende	Wurtzite
ScSb LDA	V$_0$ ( )^3	47.43 [48.627][a]	44.17 [45.863][a]	67.27 [68.904][a]	67.98 [67.756][a]
	a ( )	5.746 [5.794][a]	3.533 [3.579][a]	6.458 [6.508][a]	4.915 [4.684][a]
	B_0 (GPa)	81.749 [73.83][a]	83.138 [76.33][a]	48.178 [46.339][a]	46.96 [49.549][a]
	$B_0^`$	2.962 [3.605][a]	3.449 [3.671][a]	4.0199 [3.392][a]	3.966 [2.6244][a]
	u				0.374 [0.376][a]
	c/a				1.587 [1.5223][a]
ScSb GGA	V$_0$ ( )^3	47.49	44.22	75.32	68.066
	a ( )	5.748	3.536	6.459	4.7
	B_0 (GPa)	77.499	81.519	48.5	47.0232
	$B_0^`$	4.2374	3.5008	4.4102	4.2125
	u				0.375
	c/a				1.489

[a] Reference[8]

$V_0 = a^3/4, a^3/4, a^3$ and ½[$a^2 c(3/4)^{1/2}$] for zincblende,rocksalt,CsCl and wurtzite phases respectively.

Using these minimization curves, the equilibrium volume, the equilibrium lattice constant, the bulk modulus B_0 and its derivative have been calculated by fitting to the Murnganan equation of state, the results are summarized in Table 4.5 .Our values in a good agreement with the results of *Tabboune et al* [8].

4.2.2 Transition Pressure

The forces that act on the nuclei causes optimization of the unit cells which means that the lattice parameters change into new values and this causes the structure to come into new structure . This happens at embedded pressure with certain values called the transition pressure.

The pressure value for the structural phase transition P_t was determined by the common tangent, which is the derivative of the total energy with respect to the volume:

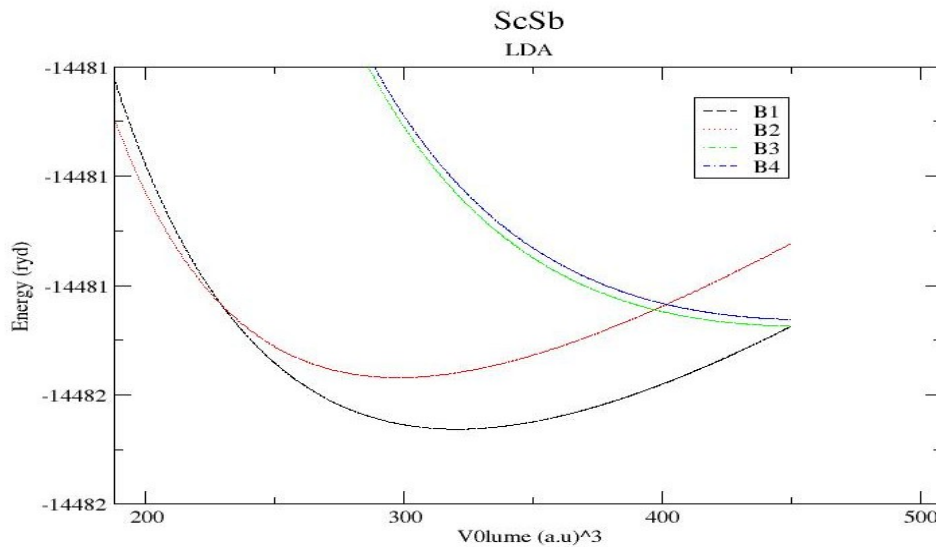$$P_t = - \frac{\Delta E}{\Delta V} \qquad\qquad (4.1)$$

Figure (4.3a): The EOS for RS, CsCl, ZB and WZ structures for ScSb using LDA method
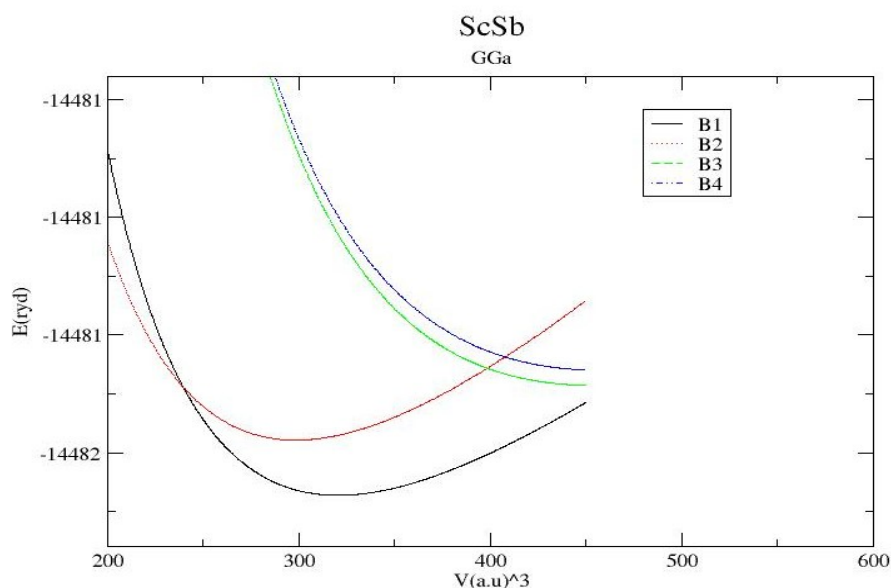
Figure (4.3b): The EOS for RS , CsCl , ZB and WZ structures for ScSb using GGA method

The transition from rocksalt phase to cesium chloride phase is occured and the pressure was found to be as shown in Table (4.6)

Table (4.6) The value of transition pressure for ScSb in LDA and GGA method.

Method	Present(RS to CsCl)	Others [a]	Experiment value[b]
LDA(GPa)	31.58	87.75	28-43
GGA(GPa)	35.4		

[a] Reference[8]

[b] Reference [10]

Our calculations show that the ground state configuration of this compound is the rocksalt structure. Nevertheless, depending on the pressure, the CsCl phase can be formed, because the curve corresponding to the RS structure cross the curve of CsCl structure. Our values(31.58 GPa, 35.4 GPa) are in a good agreement with Experimental value(28-43 GPa) of Reference [10].

4.2.3 Band Structure

The energy band structures are calculated for each structure of ScSb compound, the energy band gap gave us an idea about the behavior of the compound where it is a metal, semiconductor or insulator.

The electronic band structure of a solid describes ranges of energy that an electron can have forbidden or allowed.

A very interesting result we have obtained is that ScSb is found to be wide and direct bandgap semiconductors in the zincblende phase and wurtzite phase .
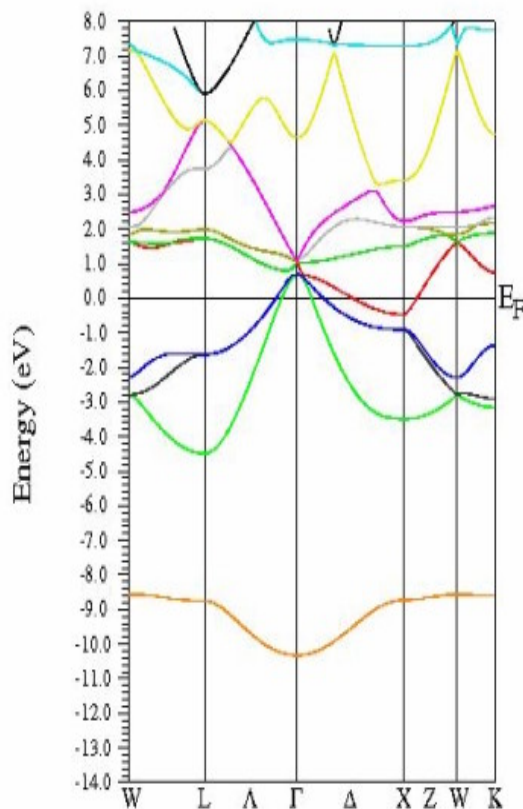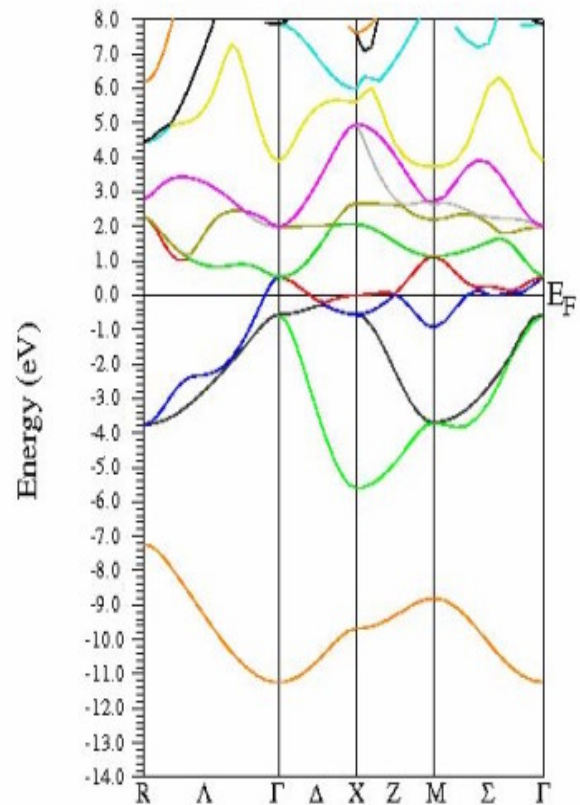

Fig (4.4a): Band structure for ScSb in the rocksalt structure

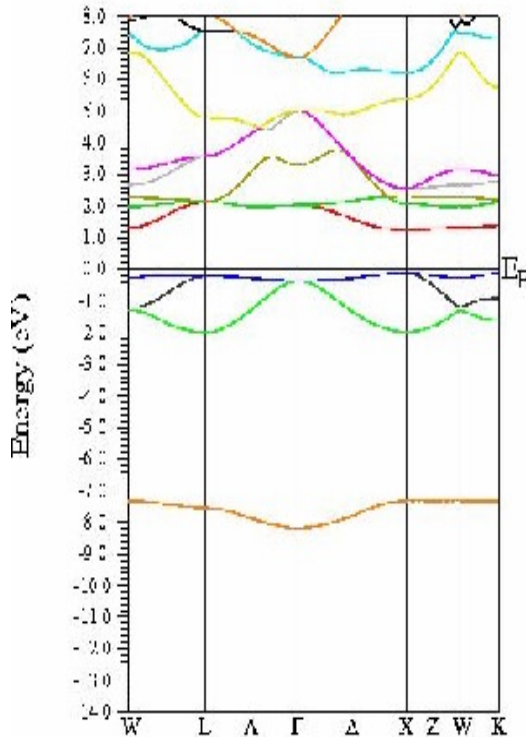**Fig(4.4b): Band structure for ScSb in the cesium chloride structure**

Fig (4.4c): Band structure for ScSb in the zincblende structure
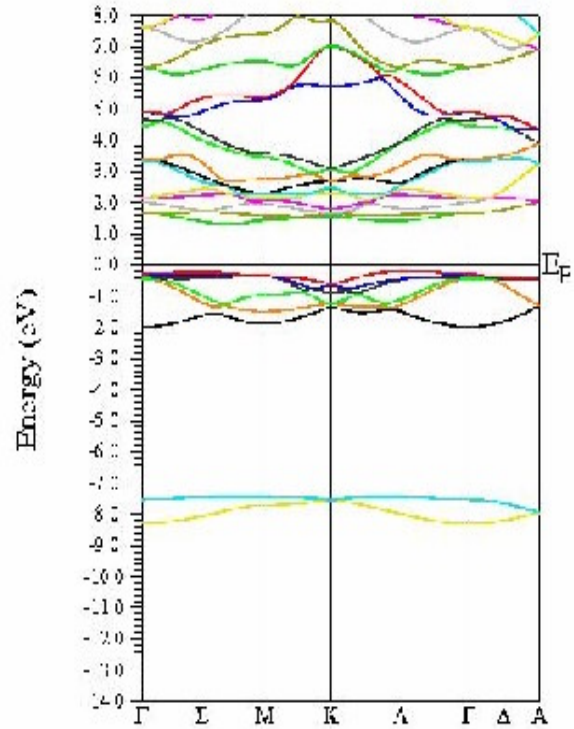
Fig (4.4d): Band structure for ScSb in the wurtzite structure

Table (4.7) Energy band gap for ScSb for four phases.

ScSb	
Phase	Energy gap (eV)
Rocksalt	-0.873
CsCl	-0.683
ZB	1.434
WZ	1.481

Table (4.7) shows the energy band gap for ScSb in RS, CsCl, ZB and WZ phases respectively, where ScSb behaves as a semimetal in rocksalt and cesium chloride phases and semiconductor in both zincblende and wurtzite phases.

4.3 ScP Compound

For this compound the same procedures have been done as for compound (ScSb), the lattice constant(a) for each structure of this

compound (RS, ZB, CsCl and WZ), the transition pressure from phase to phase and the energy bandgap for each structure have been calculated to determine whether this compound is a metal, semimetal, semiconductor or insulater by GGA approximation .

4.3.1 Optimization

The same procedures are used for ScP. We have calculated u, c/a and lattice parameter a and c for wurtzite, zincblende, rocksalt and cesium-chloride structures.

Table (4.8):Structural parameters of ScSb in the four phases((RS,CsCl,ZB,WZ where V_0 is the equilibrium volume, a is the lattice constant,B_0 is the bulk modulus and $B_0^{`}$ is the pressure derivative

Compound	Paremeters	Rocksalt	CsCl	Zincblende	Wurtzite
ScP LDA	V_0 (^{3})	35.41 [38.36][a]	33.16 [37.18][a]	49.35[51.301][a]	50.44 [51.448][a]
	a ( )	5.212 [5.35][a]	3.207 [3.338][a]	5.823[5.898][a]	4.808 [4496][a]
	B_0 (GPa)	112.334 [111.1][a]	113.9 [112.68][a]	67.62 [65.463][a]	66.86 [59.253][a]
	$B_0^{`}$	4.214 [2.903][a]	2.741 [2.849][a]	5.050 [3.247][a]	3.809 [3.520][a]
	u				0.382 [0.373][a]
	c/a				1.258 [1.30764][a]
ScP GGA	V_0 (^{3})	37.71	33.15	52.46	56.04
	a ( )	5.323	3.207	5.944	4.885
	B_0 (GPa)	102.6	115.8	59.35	56.91
	$B_0^{`}$	4.986	4.627	4.568	4.157
	u				0.382
	c/a				1.33333

[a]Reference [8]

4.3.2 Transition Phases:

Fig (4.6) shows the EOS for RS, CsCl, ZB and WZ structures using LDA and GGA methods respectively.
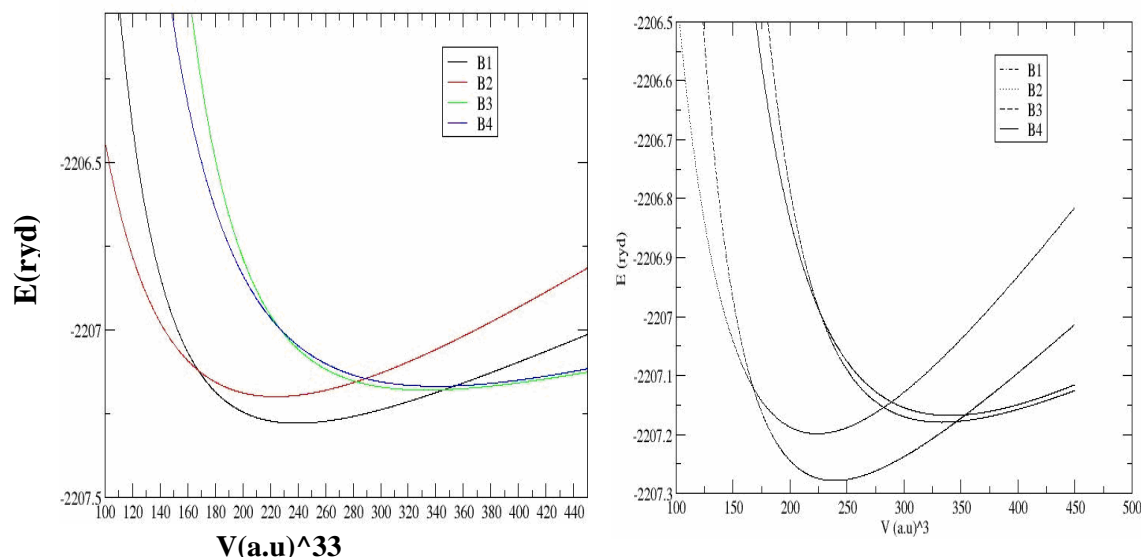

Fig 4.5a: Energy versus volume for **Fig 4.5b: Energy versus volume for**
    ScP using LDA method for the four phases   **ScP usingGGA for the four phases**

Table (4.9): the value of transition pressure for ScP in LDA and GGA method.

Method	Present	Others [a]
LDA	(RS to CsCl)=69 GPa (WZ to ZB) =84 GPa	[330 GPa]
GGA	(RS to CsCl) =73.4 GPa (WZ to ZB) =88 GPa	

a) Reference [8]

There is a difference between my calculations and *Tabboune et al*[8] especially in transition pressure from the RS phase to CsCl phase. In the present calculation, it is found that the transition pressures are 69 GPa and 73.4 GPa for ScP using respectively LDA and GGA methods, but when I calculate the transition pressure from their paper, I found it is equal to (75.55 GPa) which is in good agreement with my calculations.

4.3.3 Band structure

The same procedure was done for ScP compound in order to calculate the energy band structure for all phases.
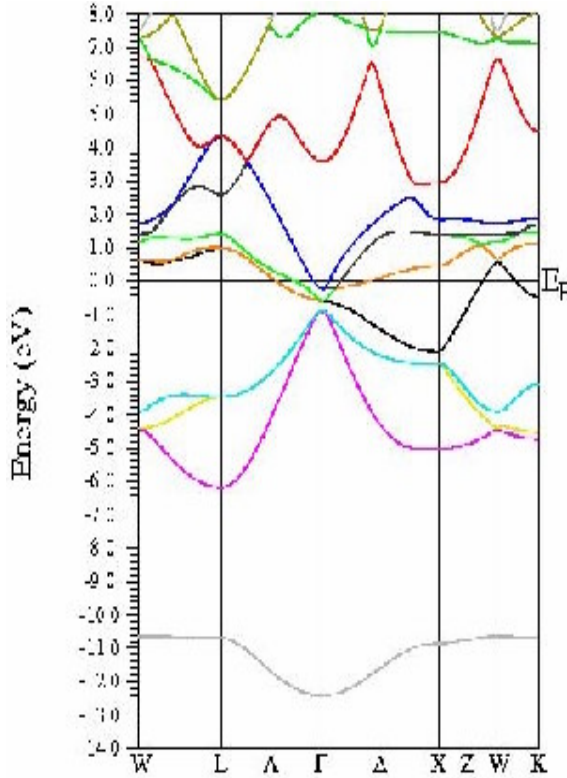

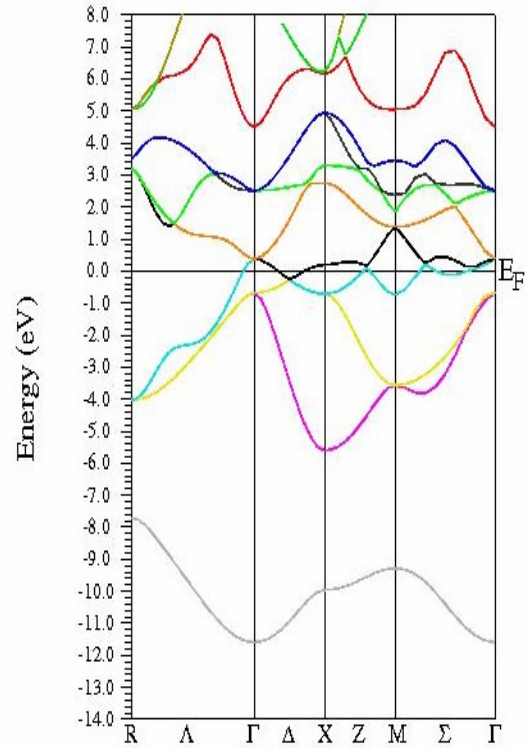**Fig (4.6a): Band structure for ScP in the rocksalt structure**

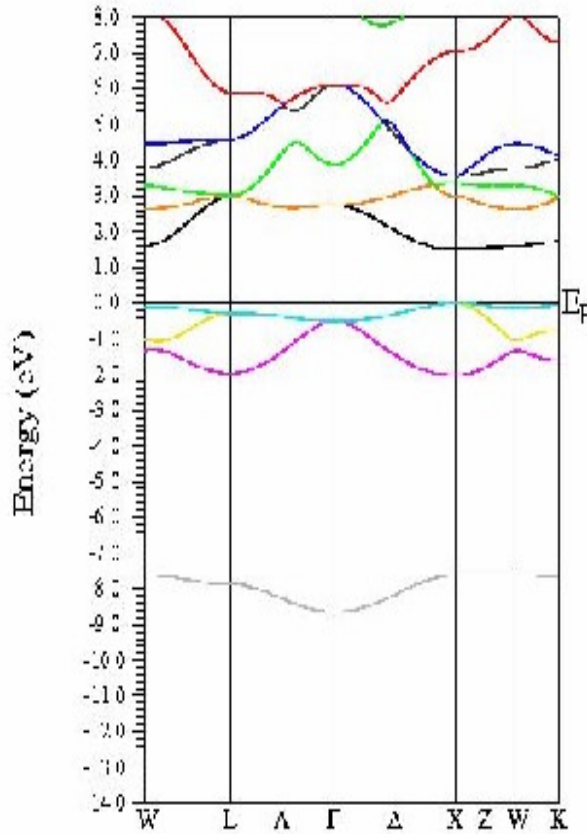**Fig (4.6b): Band structure for ScP in the cesium chloride structure**

Fig (4.6c): Band structure for ScP in the zincblende structure
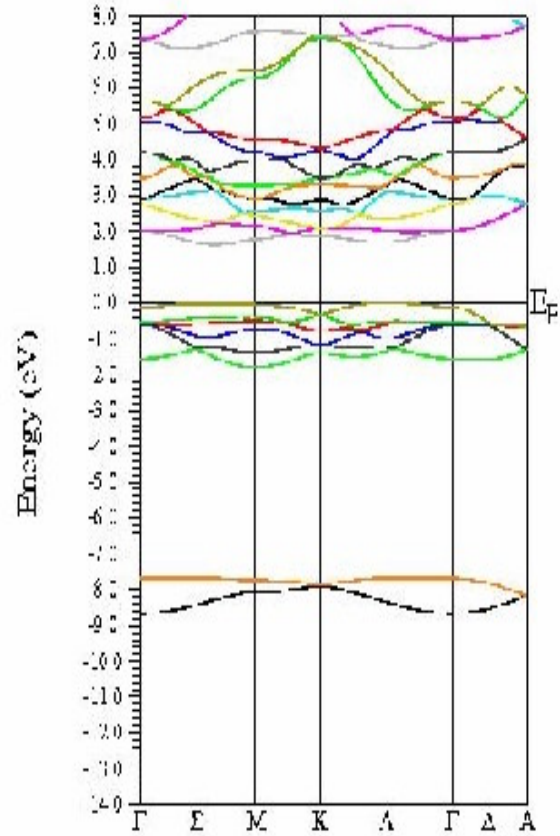
Fig (4.6d): Band structure for ScP the in wurtzite structure

Table (4.10): The energy band gap for ScP in RS,CsCl,ZB and WZ respectively

.ScP	
Phase	Energy gap (eV)
Rocksalt	-0.787
CsCl	-0.583
ZB	1.578
WZ	1.6249

Table (4.10) shows the energy band gap for ScP in RS,CsCl,ZB and WZ phases respectively, where ScP behaves as a semimetal in rocksalt and cesium chloride phases and semiconductor in both zincblende and wurtzite phases.

We found some harmony in our results (lattice parameter) compared to *Tabboune et al* results [8]. Because of the availability of some

experimental results mainly, transition pressure for ScSb (28-43)GPa[10], our results were within the range of such studies ([31.58 GPa), the thing that granted us confidence in our work taking into consideration that our method of study is different from the others, that use the first-principles full potential linear muffin-tin orbitals (FP-LMTO) method[8].

Our calculations show that the ground-state configuration of all these compounds is the rocksalt structure that agree with *Tabboune et al* results[8].

The calculated lattice parameters and bulk modulus are in agreement with experimental and previous calculations, transition pressure for ScSb compound from RS to CsCl phase and for ScP compound from Rs to CsCl and from WZ to ZB were calculated.

It can be seen that these two compounds are semimetallic in RS and CsCl phases and semiconductor in ZB and WZ phases, for which the band structutre indicates that.

The difference between the Rocksalt and CsCl curves in ScSb compound is minimum so small that the coexistence of these two phases is expected for a range of pressures and the same for ZB and WZ in ScP compound. We notice also that the minimization curves of ScSb and ScP are comparable in the sense that the arrangement of the four phases are similar (RS then CsCl, followed by ZB then WZ) .

Chapter Five
Conclusion

The calculations have been performed by using the full potential linearized augmented plane wave (FP-LAPW) method within LDA and GGA approximations. A transition from rocksalt structure to the CsCl structure is expected for ScSb and ScP at high pressure. The zincblende and wurtzite structures are very important, in these two structures, ScSb and ScP compounds have a semiconducting behavior with wide and direct band gap. It has also been found that in some cases, these compounds have similar lattice constants, so that their combination could make possible the fabrication of heterostructures.

The main results and conclusions of this study can be summarized as follows:

1- The two compounds are found to have a rocksalt structures as a ground state .

2- The calculated structural parameters using FP-LAPW method are found to be in good agreement with the available experimental data[10] and other results[8] that done by using first principle full potential linear Muffin-tin orbitals method(FP-LMTO).

3-The phase transition for ScSb compound occur from rocksalt to CsCl . The transition pressure from RS to CsCl was found to be 31.58GPa for LDA and 35.4 GPa for GGA.

4-For ScP the phase transition occur from RS to CsCl and from WZ to ZB, the transition pressure was found to be 69GPa from RS to CsCl for LDA, 73.4 GPa for GGA, and from WZ to ZB for LDA 84 GPa, 88 GPa for GGA.

5-The energy band gap for ScSb compound was calculated for RS,CsCl,ZB and WZ, it was found to be -0.873 eV, -0.683 eV, 1.434 eV and 1.48 eV respectively.

6- The energy band gap for ScP compound was calculated for RS, CsCl, ZB and WZ,, it was found to be -0.787eV, -0.583 eV, 1.578 eV and 1.6249 eV respectively.

7- This study shows that ScSb compound is semimetal in rocksalt and CsCl phases, but semiconductor in zincblende and wurtzite phases.

8- This study also shows that ScP compound is semimetal in rocksalt and in CsCl phases, but semiconductor in zincblende and wurtzite phases .

References

[1] Bouhemadu, A. (2007). **Physics Letters. A 362, 476-47.**

[2] Maachou, A. (2007) .**Physics. B 388, 384-389**.

[3] Yim, W. and Paff, R . (1974). **Physics.B45, 1456** .

[4] Van Camp, P. E. Van Doren, V.E and Devreese, J.T. (1991). **Physical Review. B44, 9056** .

[5] Van Camp,P.E. Van Doren, V.E. and Devreese, J.T. (1992). **Solid State Commmunications.81,23 .**

[6] Munoz, A and Kunc, K. (1991). **Physical Review.B44,10372**.

[7] **www.webelements.com**

[8] Tabboune, A. Rached, D. Benzair, A. Sekkal, N.and Belbachir, A. (2006). **Physica Status Solidi (B), 243, 2788-2795**

[9] Amrani, B. Maachou, A. and Driz, M. (2007**P**hysica **B: Condensed Matter 17, 384-389 .**

[10] Hayashi, J. Shirotani, I. Herano, K. Ishimatsu, N. Shimemura, S (2003) . **Solid State Communications 125 ,543-546.**

[11] Xue, W. Yu, Y. Zhao, Y. Han, H. and Gao, T. (2009). **Computational Materials Science, 46, 261-266**

[12] Schwarz, K. Blaha, P. and Madsen, G.K.H. (2002). **Computational Physics Communications. 147, 71 – 76 .**

[13] Parr, R.G. and Yang, W. (1989)**Density Functional Theory of atoms and Molecules**,(Oxford University Press, Oxford).

[14] El Haj Hassan, F. and Akbarzadeh, H. (2006). **Computational Materials Science 38,362-368.**

[15] Slater,J.C.(1930).**Physics Review.35,210.**

[16] Coulson, C. R.(1960). **Modern Physics.32,170.**

[17] Stampfl, C. Asahi, R. and Freeman, A. J. (2002). **Physical Review .B 65,161204.**

[18] Zaloni, Z. and Barth, U.(2007)**.Condensed matter Physics. 1706,10066**

[19] Benali, K.M. (2004).**First-Principles Study of Structural, Elastic and Electronic Properties of AlN and GaN semiconductors under Pressure Effect and Magnetism in AlN,** Doctorate thesis, Abou-Bakr Belkaid University.

[20] Fiolhais,C. Nogueira, F. and Marques M. **(2003)**. **A Primer in Density Functional Theory (Springer-Verlag).**

[21] San-Miguel, A. Polian, A., Guethier M.and Itie J.P. (1994) **Physical Review. B 73,1805**

[22] Hasse, M.A. Qui L. Depuydt, J. Luo H. Samarath N. and Furdyana J.K. (1993).**Appllied Physics Letters.62,2462**.

[23] Kohn, W. Vashishta, P. (1983).`**Theory of the inhomogenous electron gas'**, ed. S.Lundquist, N. H. Marck (New York, Plenum)

[24] Hohenberg, P. and Kohn, N. (1964). **Physical Review. B 864,136.**

[25] Farrer, N. and Bellaiche L. (2002). **Physical Review. B66, 201203**.
[26]Takeuchi, N. (2002). **Physical Review B, 56,045204** .

[27] Predew, J.P. Burke, K. and Emzerhof ,M. (1992). **Physical Review, B45,13244.**

[28] Blaha, P. Schwarz, K. and Luitz, J.(1999).**WEIN97**:**A Full Potential Linearized Augmented Plane Wave Pacckage for calculating Crystal Properties.** (Karlhienz Schwarz, Techn. University at Wien. Austria).

[29] Andersen, O.K. (1975). **Physical Review. B 12,3060** .

[30] Ernzerhof, M. and Scuseria, G.E. (1999). Journal Chemistry Physics.110,5029.

[31] **Ali Omar,** M. (1975). Elementary Solid State Physics: Principles and Applications, Puplished by **Addison-Wesley**

[32] Pillai, S.O. (2003). Solid State Physics , Fifth edition, Puplished by K.K.Gupta for New Age International (P) Ltd.,4835/24.

[33] Kittel, C. (1976) **Introduction to Solid State Physics**, Sixth Edition, Puplished by John Wiley and Sons, printed in USA QC176.K5.

[34] Predew, J.P. Kurth, S . Zupan, A. and Blaha, P.(1999). **Physical Review Letters.82,2544** .

[35] Tao, J. Predew, J.P. Staroverov, V.N .and Scuseria G.E. (2003). **Physical Review Letters.91,146401**.

[36] Kolling, D. Harmon .B, (1977). **Solid state Physics. 10 3107-3114 .**

[37] **http://www.en.wikipedial.org/wiki/Crystal-structure.**

[38] Ashcroft. **Solid State Physics**, (1976). New addition number 1,Puplished by. Cengage Learning (Thompson).

[39] Schwarz, K. Blaha, P. and. Madsen, G.K.H(2002). **Computational Physics Communications. 147, 71 – 76 .**

[40] Weinert, M. Wimmer, E. and Freeman , (1982). **Journal Physical Review.B26,4571-4578.**

[41] Iglesias, M. Schwarz, K. Blaha, P and Baldomir, D. (2001). **Physics Chemistry Minerals 28,67-75 .**

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الخصائص الالكترونية والتركيبية لمركبي اسكانديوم انتمونايد وسكانديوم فوسفايد تحت تأثير ضغط عالي

إعداد

هاني غالب يوسف نجي

إشراف

د. محمد أبو جعفر

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ب

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الملخص

تم استخدام اسلوب الجهد المزيد والتام ذو الموجات المستوية الخطية والذي يعتمد بدوره على نظرية توزيع كثافة الشحنات داخل الفلزات والتي يستخدم فيها اكثر من اسلوب تقريبي مثل (LDA) و (GGA) في دراسة مركب ScSb . تم حساب معادلة الحالة لكل التراكيب الممكنة مثل rocksalt, cesium chloride, zincblende, wurtzite, وتم تحديد ابعاد البلورة لكل تركيب وحساب الحجم والضغط الذي تتكون عنده كل بلورة ومن ثم تم حساب الضغط الانتقالي والذي يتحول عنده تركيب موجود الى تركيب اخر مثل الانتقال من تركيب rocksalt الى تركيب cesium chloride . تم ايضا حساب طاقة الفجوة لكل تركيب من التراكيب المذكورة حيث وجد انها تتراوح ما بين (1.48-0) الكترون فولت مما يعني أن هذا المركب قد يكون موصلاً أو شبه موصل.

بنفس الطريقة تم دراسة مركب ScP حيث تم تحديد الانتقال التركيبي وحساب الضغط الانتقالي من تركيب rocksalt الى تركيب cesium chloride ومن تركيب wurtzite الـى تركيب zincbende ، وقد تم حساب معادلة الحالة لكل من التراكيب السابقة وتم تحديد ابعاد البلورة في كل حالة وحساب طاقة الفجوة حيث تبين ان طاقة الفجوة لهذا المركب تتراوح ما بين (1.6249-0) الكترون فولت مما يعني ان هذا المركب قد يكون موصلاً أو شبه موصل.

من الدراسة السابقة استطعنا الحصول على النتائج التالية:

1. ان الحسابات التي حصلنا عليها تتطابق بشكل كبير مع الحسابات السابقة النظرية والتجريبية.

2. في مركب ScSb، تم الانتقال من تركيبrocksalt   الى تركيب كلوريد السيزيوم cesium chlorideعند ضغط عالي مقداره 31.5 جيجا باسكال باستخدام طريقة LDA و35.4 جيجا باسكال باستخدام طريقة GGA.

3. في مركب ScP، تم الانتقال ايضا من تركيب rocksalt الى تركيب كلوريد السيزيوم (cesium chloride) عند ضغط عالي مقداره 69 جيجا باسكال باستخدام طريقة LDA ، و73.4 جيجا باسكال باستخدام طريقة GGA، كما تم ايضا الانتقال من تركيب wurtziteالى تركيب zincblende عند ضغط عالي مقداره 84 جيجا باسكال باستخدام طريقة LDA، و 88 جيجا باسكال باستخدام طريقة GGA.

4. من حساب طاقة الفجوة تبين ان مركب ScSb يسلك سلوك اشباه المعادن في تركيب ال rocksalt وسلوك المعادن في تركيب كلوريد السيزيوم cesiumchloride وسلوك اشباه الموصلات في تراكيب ال zincblende و wurtzite باستخدام طريقتي LDAو GGA.

5. من حساب طاقة الفجوة تبين ايضا ان مركب ScP يسلك سلوك اشباه المعادن في تركيب ال rocksalt وسلوك المعادن في تركيب كلوريد السيزيوم cesiumchloride واشباه الموصلات في تركيبي zincblende و wurtzite باستخدام طريقتي LDA و GGA.

6. تركيب rocksalt هو التركيب الاساسي والطبيعي لمركبي ScSb و ScP تحت الظروف العادية.