An-Najah-National University

Faculty of Graduate studies

Structural, Electronic, Elastic & Optical Properties of SrRhO₃, SrZrO3and SrTiO₃ Compounds: FP-LAPW Study

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Dedicated

I do dedicate this work to my mother, father, husband and my son laith. They help me and give me a big support.

Acknowledgment

I do thank Allah and each one who helps me and gives me an encouragement and support to finish this thesis successfully.My deepest appreciation to my dear supervisor, Dr. Mohammed Abu Jafar for his guidance, helpand advices throughout research work and writing up the thesis.

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v الإقرار

انا الموقع ادناه مقدم الرسالة التي تحمل العنوان :

Structural, Electronic, Elastic &Optical Properties of SrRhO₃,SrZrO₃ and SrTiO₃ Compounds: FP-LAPW Study

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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.

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By

AreejMaroof A. Shawahne Supervisor Dr.Mohammed S. Abu-Jafar Abstract

He structuralelectronic, elastic and opticalproperties of cubic perovskite SrTMO3 (TM=Zr,Rh,Ti) have been examined by utilizing the full potential linearized augmented plane wave (FP-LAPW),Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA)and local density approximation(LDA) in the framework of the density functional theory . The modified Becke-Johnson potential (mBJ) has been used to improve the energy band gap for the compounds. Structural parameters (lattice parameters, bulk modulus and first pressure derivatives) have been investigated and found to be in good agreement with other experimental and theoretical results.

The present calculationsare found to be in good agreement with the available experimental data and other theoretical results.SrRhO₃compound is found to behave as metallic, while SrZrO₃ and SrTiO₃compound behave as insulator and semiconductor, respectively.SrRhO₃compound has been found in ductile nature while SrZrO₃and SrTiO₃compounds have brittle nature. In addition, SrRhO₃compound has ionic bond while SrZrO₃and SrTiO₃compounds have covalent bonds. Finally, SrRhO₃compound has greater dielectric constant than SrZrO₃ and SrTiO₃compounds.



Chapter 1 Introduction

Perovskite structure solids have a great interest in materials science since the relatively simple crystal structure has many optical, catalytic, diverse electric, magnetic, and magneto resistive properties [1].These materials that are very often used as sensor catalytic electrodes in fuel cells are also considered promising candidates for optoelectronics [2]. Recently, a lot of attention, in the researches on experimental and theoretical fronts, has been focused on perovskite oxides RE–TM–O₃ (RE indicates rare earth while TM refers to transition metal elements) [3,4,5,6,7].

Perovskites with transition metal ions (TM) demonstrates enormous wide variety of electronic or magnetic properties. Transition metal oxides are widely used in the technological applications such as catalysis, microelectronics, substrates for the development of high Tc superconductors, gas sensors, and thin films of cubic SrTMO3 perovskite.

The provoskite structure of $A^{2+}B^{4+}O_3^{2-}$ with the oxygen in the face center [8]. Provoskite structure has been found out in the Ural mountains of Russia by Gustav Rose in 1839 and it is named after Russian mineralogist L.A.Provoski (1792–1856)[9]. Transition metal oxides SrTMO₃ crystallize in the ABO₃ cubic perovskite crystal structure of space group Pm-3m (221), where A atom is larger than B and O is anion. The TM atom (transition metal) sits at body center position (1/2, 1/2, 1/2), Sr atom (alkaline earth or rare earth element) stands at cube corner positions (0, 0,

0), and oxygen atoms locate at face centered positions (1/2, 1/2, 0), (0,1/2,1/2) and (1/2,0,1/2). A large number of metallic elements are stable in the perovskite structure, if the tolerance factor *t* is in the range of 0.75 – 1.0[10]. The ratio of the two expressions for the cell length is called the Goldschmidt's tolerance factor *t* and allows us to estimate the degree of distortion. It is based on ionic radii where (r_A , r_B , and r_O) are ionic radii as described in equation (1.1)[11]:

$$t = \frac{(r_{A+}r_{O})}{\sqrt{2(r_{B+}r_{O})}} (1.1)$$

The crystal structure of SrTMO₃ (TM=Rh,Zr,Ti) is shown in Figure 1.1



Fig.1.1: The crystal structure of SrTMO₃ (TM=Rh, Zr,Ti).

Crystals of perovskite appear as cubic, but are crystallize in the orthorhombicsystem. Perovskites have many colors like black, gray, orange and yellow.

SrTMO₃ is defined as Sr^{+2} and O^{-2} ions forming a cubic close packed lattice with TM (Rh, Ti, Zr) ions filling the octahedral gabs made by the oxygen. The perovskite structure has a three dimensional net of corner sharing

[TMO6] octahedra with Sr2+ions in the twelvefold cavities in between the polyhedral [11].

Material science is interested in physical properties of pervoskite includemagneto resistance, ionic conductivity, superconductivity and a multitude of dielectric properties, which have great importance in microelectronics and telecommunication. Provoskite has much application in photovoltaic, laser, light emitting diodes and Photo electrolysis.

Some scientists studied the properties of perovskite structure like elastic, electronic, optical properties and compare their results with the experimental and other theoretical results [12, 13, 14,15,16,]. In 1992, Roosmalen*et al.* studied the structure of SrZrO₃ [17]. In 2003, Mete *et al.* studied the electronic and structural properties of SrZrO₃ and SrTiO₃pervoskite [18]. They calculated lattice parameter and bulk modulus. On the other hand, they predicted that SrTiO₃ is semiconductor with direct band gap (1.92 eV) and SrZrO₃ is insulator with indirect band gap (3.37 eV) between Γ and R points. In 2009, Baudali*et al.*[19] studied structural, optical, electronic and thermal properties of SrTiO₃pervoskite cubic structure by usingthefull-potential linearized augmented plane wave(FP-LAPW)method [20].

In 2011, Daga*et al.* used the first principle to study the cubic SrMO₃ (M=Ti, Zr, Mo, Rh, Ru)compounds and calculated its lattice parameters. The lattice parameters of SrRhO₃, SrZrO₃ and SrTiO₃ in perovskite structure are 3.932, 4.076 and $3.911A^{\circ}$, respectively [21].

In 2016, Ali et al. [22] used CASTEP code [23] (CASTEP is a quantum mechanics-based program designed specifically for solid-state materials science. CASTEP employs the density functional theory plane-wave peseudopotential method, which allows you to perform first-principle quantum mechanics calculation that explores the properties of crystals. Peseudopotential were used to describe the interaction of ionic core and valence core), to study the structural, elastic and optical properties of $SrTMO_3$ (TM= Rh, Mo, Ti, Zr) under pressure. They predicted that $SrTiO_3$ and SrZrO₃ have a brittle nature, while SrMoO₃ and SrRhO₃ have a ductile nature. Also, they concluded that SrRhO₃ has the highest dielectric constant among them. Also, they concluded that SrRhO₃ has the highest dielectric constant among them. On the other hand, they predicted that the highest value of young modulus indicated the presence of covalent bond and the young modulus increases with increasing pressure. In this work, we studied the electronic, structural, elastic and optical properties of SrTMO₃ (TM=Rh, Zr) by using FP-LAPW method. The motivation of this work is to improve the calculations using all electron method (FP-LAPW) method. For band Structure, the energy band gapis an energy range in a solid where no electron states can exist. In graphs of the electronic bandstructure of solids, the band gap generally refers to the energy difference (in electron volts) between the top of the valence band and the bottom of the conduction band in insulators and semiconductors.

In this study, we are going to use (FP-LAPW) method was used to study the electronic, optical, elastic and structural properties of the three transition oxide SrTMO₃(TM=Ti, Zr, Rh). For optical properties we are going to calculate dielectric constant (real part is related to the polarization of the charge inside the solid and it describes the ability to store the charge, while the imaginary part describe the absorption behavior and transition of the electrons from band to band), refractive index is a dimensionless number that describes how light propagates through the medium and it is equal to the ratio between the speed of light and the phase velocity, while extinct factor describes the absorption behavior, Reflectivity is the fraction of incident electromagnetic power that is reflected at an interface, energy loss function is describing the energy loss of the photon propagates inside the material and when electron absorb this energy, it moves from valence band to conduction band, conductivitydescribes the absorption behavior and transition of the electrons from valence band to conduction band.

Chapter 2 Methodology

Schrödinger equation for a N-body system is a very hard process to be solve. It is clear that it is necessary to involve some approximations to face the many body problem

H is the Hamiltonian function, the first term is the kinetic energy operator represents the nuclei (T_n) , the second is for the electrons (T_e) . The finalthree term show the coulomb interaction between electron and nuclei (V_{en}) , betweenelctron and others electrons (V_{ee}) , and between nuclei and other nuclei (V_{nn}) .

There isn't an exact solution to this Schrodinger equation. Historically, there are a series of approximations which are very important to solve this problem.

These approximations are:

2.1 The Born-Oppenheimer approximation

Since the early days of quantum mechanics, the adiabatic Born– Oppenheimer approximation (ABO) is consider the standard ansatz to explain the interaction between electrons and nuclei[24, 25]

It suggests that the lighter electrons cop adiabatically with the motion of the heavier nuclei, while they remain at any time in their instantaneous ground state [26]. This approximation assume that the nuclei are more massive than electrons and it has zero kinetic energy because of that we can neglect the movement of nuclei when we compare with an electron, the first term in Schrödinger equation are omitted and the final[27] term kept constant, new equation becomes:

 $H = T_e + V_{ee} + V_{ext}(2.2)$

 T_e is the kinetic energy of electron gas, V_{ee} is the potential-energy between electron-electron interactions, V_{ext} is the potential energy of the electrons in the potential of the nuclei.

The complex many-particle problem represented in the V_{ee} term.

2.2Hartree-Fock Approximation

In Hatree-Fock approximation, the many-particle system solved by assuming that the electrons are independent of each other.

The wave function of electrons can be written as:

$$\Psi(\mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{3},...,\mathbf{r}_{N}) = \Psi_{1}(\mathbf{r}_{1})\Psi_{2}(\mathbf{r}_{2})\Psi_{3}(\mathbf{r}_{3})....\Psi_{N}(\mathbf{r}_{N})$$
(2.3)

The Ψ_n (r_n) is the wave function for the electrons, the total Hamiltonian can be written as:

$$(T_s + V_{ext} + V_H) \Psi(r) = E \Psi(r)$$
(2.4)

were the T_s is the kinetic energy and V_{ext} is the external potential and the V_H is the Hattree potential for non-interacting electrons V_H can be written as :

$$V_{H} = \frac{1}{8\pi\varepsilon_{0}} \sum_{ij} \frac{|\psi(r_{i})|^{2} |\psi(r_{j})|^{2} d^{3}r_{i} d^{3}r_{j}}{|\vec{r_{i}} - \vec{r_{j}}|}$$
(2.5)

This technique has vast computational effort, which makes it more complicated system and this is the big problem.

2.3 Density function theory

Density functional theory is more modern and strong than Hatree-Fock (HF) approximation. Density functional theory replace the many-body electronic wave function with the electronic density as the basic quantity attempting to address both the high computational demands of post-HF and the inaccuracy of HF methods [28,29].DFT has been founded in 1964 by two theorems due to Hohenberg and Kohn. DFT provides a way to solve many-body problem onto a single-body problem (non-interacting system that has the same total density).

Modern DFT bases on two theorems by Hohenberg and Kohn [30]. The first theorem indicates that the groundstate electron density determines the electronic wave function uniquely and hence all ground-state properties of an electronic system [31]. Hohenberg and Kohn can reduce the 3N spatial to 3 spatial coordinates in Schrödinger equation. The second theorem states that the successful minimizing of the energy functional will produce the ground state density ρ_0 . The lagrangian of undetermined multiples can be applied to solve the variation problem of minimizing the energy functional $E(\rho)$.

The Born Oppenhamiar approximation is solved the Schrödinger equation but the problem is still exist (many electron system). The DFT is trying to solve this problem by Hohenberg and Kohn equation.

In DFT, the key variable is the electron density n (r) which for a normalized Ψ

is explained by:

$$n(\mathbf{r}) = N_e \sum_{s_1} \cdots \sum_{s_{N_e}} \int d\mathbf{r}_2 \cdots d\mathbf{r}_{N_e} \left| \Psi(\mathbf{r}, s_1, \mathbf{r}_2, s_2, \dots, \mathbf{r}_{N_e}, s_{N_e}) \right|^2$$
(2.6)

For a given ground state density ρ_0 it is possible to work out the ground state wave function $\Psi(r1,...,r_N)$ [32]. In other word, the Ψ is a unique function of ρ_0 [33]:

 $\Psi_0 = \Psi(\rho_0)$

The ground-state energy is a functional of $\rho_{0:}$

$$E_0 = E[\rho_0] = \langle \Psi(\rho_0) I T + V + U I \Psi(\rho_0) \rangle$$
 (2.7)

Where T is the kinetic energy of single electron, V is external potential and U is e-e interaction.

The contribution of the external potential is represented by $\langle \Psi(\rho_0) | V | \Psi(\rho_0) \rangle$

It is possible to write the external potential n term of ρ_0

$$V[\rho_0] = \int V(r) \rho_0(\vec{r}) d^3r$$
 (2.8)

Moreover, it is also possible to write the contribution of the external potentialas density,

$$V[\rho] = \int V(\vec{r}) \rho(\vec{r}) d^3r \qquad (2.9)$$

While V[n] is called non-universal functional, the functional T[ρ] and U[ρ] are called universal functional .

Having specified system, i.e., having defined \hat{V} , one then has to minimize the functional

$$E[\rho] = T[\rho] + U[\rho] + V[\rho] = \int V(\vec{r}) \rho(\vec{r}) d^3r \qquad (2.10)$$

Reducing energyfunction will produce the ground state density ρ_0 and thus all other ground state observables.

The Lagrangian method of undetermined multipliers [34] can help us to solve the variation problems of minimizing the energy functional. We considered that energy functional doesn't have an electron-electron interaction.

$$\left[-\frac{\hbar^2}{2m_0}\vec{\nabla}_i^2 + \mathrm{Vs}(\vec{r})\right]\Psi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r}) \qquad (2.11)$$

Where the orbital $\phi_i(\vec{r})$ reproduces the density $\rho(\vec{r})$ of the authentic manybody system

$$\rho(\vec{r}) = \rho_{s}(\vec{r}) = \sum_{i=1}^{N} |\phi_{i}(\vec{r})|^{2}$$
(2.12)

The effective single-particle potential can be written in more detail as

$$Vs(\vec{r}) = V(\vec{r}) + e^2 \int \frac{\rho(\vec{r'})}{|\vec{r} - \vec{r'}|} d\vec{r'} + V_{xc}[\rho_s(\vec{r})](2.13)$$

Where the second term is Hatree expression portraying the electronelectron Coulomb repulsion and V_{xc} is the exchange correlation possibility.

2.4 Single particle Kohn-Sham equation

The LAPW method is a procedure that is used for solving the Kohn-Sham equations of the ground state density, total energy, and (Kohn-Sham) Eigen Values (energy bands) of a many-electron system.

The above expression can be explained as energy functional of a *non-interacting* classical electron gas, subject to 2 external potentials: the first one is because of the nuclei $\hat{V}_{ext}[\rho]$, and the second potential is because of exchange and correlation effects $\hat{V}_{xc}[\rho]$. The corresponding Hamiltonian - called the Kohn-Sham Hamiltonian - .

The straight forward application of this formula has two barriers:

First, the exchange-correlation energy Exc is not known precisely, and second, the kinetic term must be created in terms of the charge density.

The exact ground-state density (\vec{r}) of an N-electron system is

$$\rho(\vec{r}) = \sum_{i=1}^{N} \phi_i^*(\vec{r}) \phi_i(\vec{r}) = \sum_{i=1}^{N} |\phi_i(\vec{r})|^2$$
(2.14)

Where the single-particle wave functions $\phi_i(\vec{r})$ are the N lowest-energy solutions of the Kohn- Sham equation

$$\widehat{H}_{KS}\phi_{i} = \epsilon_{i}\phi_{i} \qquad (2.15)$$

Sometimes Kohn-Sham equation is written as:

$$\widehat{H}\phi_{i}(\vec{r}) = \left[-\frac{\hbar^{2}}{2m_{e}}\vec{\nabla}_{i}^{2} + V_{eff}\right]\phi_{i} = \epsilon_{i}\phi_{i} \qquad (2.16)$$

The \widehat{H} is commonly known as the Hamiltonian operator. The effective potential $V_{eff}(\vec{r})$ represents the sum of the external, the exchange-correlation and the Hartree (electrostatic)potentials:

$$V_{eff}(\vec{r}) = V_{ext}(\vec{r}) + \frac{\delta E_H[\rho]}{\delta \rho} + \frac{\delta E_{xc}[\rho]}{\delta \rho} = V_{ext}(\vec{r}) + \frac{e^2}{4\pi\epsilon_0} \int \frac{\rho(r')}{|\vec{r} - \vec{r}'|} d\vec{r}' + V_{xc}(\vec{r})$$

$$(2.17)$$

From above equation we conclude that the V _H and V_{xc}depend on the charge density $\rho(\vec{r})$, which in turn depends on the ϕ_i which are being searched. This shows that we are using self-consistency problems: the solution ϕ_i determine the original equation (V_H and V_{xc} in H_{ks}), it is impossible to write down and solve the equation before its solution is known. Some starting density ρ_o is guessed, and a Hamiltonian H_{KS1} can construct with it. The Eigen value problem is solved, and Φ_1 can be

determined from ρ_1 . Now ρ_1 can be used to construct H_{KS2} which will yield ρ_2 , etc. The procedure can be used until the series converge and ρ_f gets out as shown in Figure (2.1).



Figure (2.1): Flow chart of solving the self-consistent kohn-Sham equation.

2.5 The Exchange-Correlation functional.

The detailed above Kohn-Sham scheme was exact: no other approximations were made except the preceding Born-Oppenheimer approximation,. Even though we completely ignored the fact that we do not know the exchange-correlation functional. Two approximations are used to solve this unknown part. These approximations are LDA (Local Density Approximation) and GGA (Generalized Gradient Approximation). It is not possible to understand .The reasons for these approximations success well; this may be partially due to the fact that both approximations obey the sum rule for the exchange-correlation hole in the electron density [35].

2.6 Local Density Approximation (LDA)

Kohn and sham applied LDA approximation to DFT [36]. The XC functional is not identified accurately and must be approximated [37].Local density approximation can be solved the exchange-correlation energy. The local density approximation for the exchange correlation energy has the following term:

$$E_{xc}^{\text{LDA}} = \int \rho(\vec{r}) \varepsilon_{xc}[\rho(\vec{r})] d\vec{r}$$
(2.18)

Where $\varepsilon_{xc}[\rho(\vec{r})]$ indicates the exchange-correlation energy per particle of a uniform (a homogeneous) electron gas, that only based on the electrondensity $\rho(\vec{r})$.

It could be found that the exchange-correlation energy due to a particular density by dividing the material into infinitesimally small volumes with a constant density [38]. Each of such volume participates in the total exchange correlation energy with an amount equal to the exchange correlation energy of an identical volume filled with a homogeneous electron gas. The LDA assumes that the density is the same everywhere [39]. The exchange-correlation energy is decomposed into exchange and correlation terms linearly,

$$E_{xc}^{\text{LDA}} = E_x^{\text{LDA}} + E_c^{\text{LDA}}$$
(2.19)The first term is

the exchange energy that related to Pauli Exclusion Principle.

The second term, called the correlation energy E_c^{LDA} , originates from the interaction of electrons having the same spin [39].

Then comes the next logical step to improve the LDA calculations which is to make the exchange-correlation contribution of every infinitesimal volume dependent on the local density in that volume and on the density in the neighboring volumes (inhomogeneous of electron density). That means that the gradient of the density has a role. This approximation is called the Generalized Gradient Approximation (GGA).

2.7 Generalized Gradient Approximation (GGA)

Generalized gradient approximations (GGA's) for the exchange-correlation energy improve based on the local spin density (LSD) description of molecules, atoms, and solids [40]. Whereas LDA uses the exchange energy density of the uniform electron gas, regardless of the homogeneity of the real charge density, the generalized gradient approximation takes care of such inhomogeneities (non uniform charge density) by including the gradient of the electron density in the functional. GGA uses the gradient of the charge density $\vec{\nabla}\rho(\vec{r})$. Then the GGA can be conveniently written as follows

$$E_{xc}^{\text{GGA}} = \int \rho(\vec{r}) \varepsilon_{xc} \left[\rho(\vec{r}), \overline{\nabla} \rho(\vec{r}) \right] d\vec{r}$$
(2.20)

Where the $\rho(\vec{r})$ is the charge density and $\nabla \rho(\vec{r})$ is the gradient of the charge density.

At present, two GGA functional, one suggested by Becke and Perdew (BP) and other suggested more recently by perdew and Wang (PW), are in the most popuar ones in the leterature [41].

GGA seeks to improve upon the accuracy of the local density approximation in electronic-structure calculation.

2.8 The modified Becke-Johnson (mBJ)

The modified Becke-Johnson [42] is tested on various types of solids which are difficult to describe theoretically [43]. The BJ exchange potential has been implemented [44] self-consistently into the WIEN2K code which is based on the full-potential (linearized) augmented plane-wave and local orbital's method to solve the KS equations for periodic systems. The BJ potential improves over LDA and PBE-GGA for the description of band gaps .Further improvement has been achieved by a modified version (TBmBJ) [45] of the BJ exchange potential.

The mBJ potential are used to improve the energy band gap and electronic properties for SrTMO₃

Several groups have used (mBJ) potential for the calculation of electronic properties [46, 47].

2.9 Augmented Plane Wave (APW) method

Augmented plane wave introduced by Slater as a basis functions for solving one-electron equation. APW method is considered a procedure to solve the Kohn-Sham equation. In the APW scheme, the unit cell is partitioned into two types of regions: (I) atomic centered muffin-tin (MT) spheres with radius R_{α} , and (II) the remaining interstitial region as shown in figure (2.2).



Figure 2.2: scheme of Augmented Plane Wave.

In both types of regions, different basis sets are used. In the region far away from the nuclei, it was found that electrons are almost free so plane waves are employed. Close to the nuclei, electron behaves almost as if they were in a free atom and therefore can be described atomic like- wave function (radial solution of Schrödinger's equation)

The introduction of such a basis is due to the fact that close to the nuclei the potential and wave functions are very similar to those in an atom, while between the atoms then are smoother i.e., in the region far away from the nuclei, the electrons are more or less "free".

The APWs consist of:

$$\phi_{k_{n}}(\vec{r}, E) = \begin{cases} \frac{1}{\sqrt{V}} e^{i(k_{n}).\vec{r}}, & \vec{r} \in I \\ \sum_{l,m} A_{lm}^{\alpha,k_{n}} u_{l}^{\alpha}(r', E) Y_{m}^{l}(\hat{r}'), & r' < S_{\alpha} \end{cases}$$
(2.21)

Where $k_n = k + K_n$; K_n are the reciprocal lattice vectors and k is the wave vector inside the first Brillouin zone, V is the volume of the unit cell, the poison vector (r') inside the sphere (S_{α}) , u_{lm} is the numerical solution to the radial Schrodinger equation at the energy ϵ .

Lately, the development of the augmented plane wave (APW) techniques from slater's APW, to LAPW and APW+Lo was pottrayed by Schwarz and et al [48].

2.10 The Linearized Augmented Plane Wave (LAPW) Method

The linearized augmented plane wave method (LAPW) scheme introduced by Andersen(who recommended the expansion of energy dependence of radial wave functions u(r') inside the atomic spheres with its energy derivative $\frac{\partial u^{\alpha}(r', E)}{\partial E} = \dot{u}^{\alpha}(r', E)$, in this scheme, a linear combination of radial function times spherical harmonics are utilized.

Inside atomic sphere of radius R_M a linear combination of radial functions times spherical harmonics $Y_{lm}(r)$ is used where $u_l(r,E_l)$ is the (at the origin) regular solution of the radial Schrödinger equation for energy E_l and the spherical part of the potential inside the atomic sphere, $u^{\alpha}(r', E)$ is the energy derivative of u_l taken at the same energy E_l

$$\phi_{k_n}(\vec{r}, E) = \sum_{l,m} \left(a_{lm}^{\alpha, \vec{k} + \overline{K_n}} u_l^{\alpha}(r', E) + b_{lm}^{\alpha, \vec{k} + \overline{K_n}} \dot{u}_l^{\alpha}(r', E) \right) Y_m^l(\hat{r}'), \quad r' < R_\alpha$$
(2.22)

In the interstitial region a plane wave is used

$$\phi_{k_n}(\vec{r}, E) = \frac{1}{\sqrt{V}} e^{i(k_n).\vec{r}} , \quad \vec{r} \in I$$
(2.23)

Where *k* is the wave vector and $k_n = k + K_n$; K_n are the reciprocal lattice vectors inside the first Brillouin zone. Each plane wave is added by an atomic-like function in every atomic sphere.

The solutions to the Kohn-Sham equations are extended in this combined basis set of LAPW's based on the linear variation method [49]

$$\psi_k = \sum_n c_n \phi_{k_n}$$

The coefficients C_n are decided by the Rayleigh-Ritz variation principle. The cutoff parameter $R_{mt}K_{max}$ =6-9 controlled the union of this basis, where is the smallest atomic sphere radius in the unit cell and K_{max} represents the magnitude of the largest K vector.

2.11 The Augmented Plane Wave + local orbits (LAPW+lo) method

An alternative approach was proposed by Sjöstedt et al [50], namely the APW+lo (local orbital) method .It has been revealedthat the standard LAPW method with the additional constraint on the PWs of matching in

value and slope to the solution inside the sphere does not indicate the most efficient way to linearize Slater's APW method. It is possible to make it much more efficient when one uses the standard APW basis, but of course with $u_l(r,E_l)$ at a fixed energy E_l in order to keep the linear eigenvalue problem. One then adds a new local orbital (*lo*) to have enough variational flexibility in the radial basis functions [51]:

$$\phi_{\vec{k}_{n}} = \sum_{lm} \left[a_{lm,\vec{k}_{n}} u_{l}(r, E_{l}) \right] Y_{lm}(\hat{r})$$
(2.25)

$$\phi_{lm}^{lo} = \begin{cases} o, & \vec{r} \in I \\ \left[a_{lm}^{lo} u(r', E_{1,l}) + b_{lm}^{lo} \dot{u}_l(r', E_{1,l})\right] Y_{lm}(\hat{r}) , & r' < R_{\alpha} \end{cases}$$
(2.26)

The coefficient a_{lm}^{lo} , b_{lm}^{lo} are decided by necessities that ϕ_{lm}^{lo} should be regularized and has zero value and slope at the sphere border.

2.12 Full Potential Linearized Augmented Plane Wave (FP-LAPW) method

The *full-potential linearized augmented-plane wave* (FP-LAPW) method is commonly used to enable most accurate calculations of the magnetic properties and the electronic structure of crystals and surfaces [52].The FP-LAPW method is an all-electron algorithm which is universally applicable to all atoms of periodic table, in particular to transition metals and rare-earth and to multi-atomic system with compact as well as open structures [53].

In this study we used the full-potential linearized augmented plane wave (FP-LAPW) by using WIEN2k code to investigate the electronic, structural, elastic and optical properties of four transition oxide SrTMO₃(TM=Ti, Rh, Zr).Using FP-LAPW method, the Kohn-Sham equation can be solved, the way that used to expand the wave function into atomic orbital in spherical regions around the atomic positions, while it is expanded into plane waves in the region between the spheres .

The full- potential linearized-augmented-plane wave (FP-LAPW) method suggested by the Andersen [54] on which WIEN2k code is based.

FP-LAPW method is most accurate schemes that are used to solve Kohn-Sham equation.

The FP1-LAPW technique extends, the potential in the following form

$$V(\vec{r}) = \begin{cases} \sum_{lm} V_{lm}(r) Y_{lm}(\hat{r}), & \text{inside sphere} \\ \sum_{\vec{k}} V_{\vec{k}} e^{i\vec{k}.\vec{r}}, & \text{outside sphere} \end{cases} (2.27)$$

The entire energy is worked out according to Weinter et al. [55]. The forces on the atoms are calculated according to Yu et al [56].

It is possible to work out the Fermi energy and the Weights of each band state by using a modified tetrahedron method [57].

2.13 WIEN2k code

One successful implementation of the FP-LAPW method is WIEN2k code, a code written by Blaha, Schwarz and co-workers[58].

The program package WIEN2k allows us to perform electronic structure calculations of solids using density functional theory (DFT).

Full-potential (linearized) augmented plane wave and local-orbitals [FP-(L)APW+lo] basis set uses to solve Kohn Sham equations of density functional theory. Blaha and Karlheinz Schwarz from the Institute of Materials Chemistry of the Vienna University of Technology developed that. In DFT, the local density approximation LDA or Generalized gradient approximation GGA can be used .Wein2k represents all-electron scheme including relativistic effects has many features.

Chapter Three Computational method

The computation has been performed by using full potential linearized augmented plane wave (FP-LAPW) method within the Local density approximation (LDA) andPerdew-Burke-Ernzerhof of generalized Gradient approximation(PBE-GGA) as implement by using Wien2k code[59].The FP-LAPW method is used to calculate the electronic, structural, elastic and optical properties of SrTMO₃ (TM= Rh,Zr,Ti). The expansion of spherical harmonics is defined within a muffin-tin sphere of radius RMT around each nucleus [60]. The crystal structure of SrTMO₃(TM=Rh,Zr,Ti) can be defined by lattice parameters. Structural parameters (Lattice parameter, volume, Bulk modulus, first derivative of pressure and energy) are solved by Murnaghan equation of state [61].

In the GGA approximation, The Muffin-Tin radius R_{MT} values used are 2.5, 1.95,1.67a.u for Sr, Rh and O atoms for SrRhO₃compoundand 2.5, 1.8 and 1.5 a.u for Sr, Zr and O atoms for SrZrO₃ compound. In SrTiO₃, the R_{MT} values used are 2.36, 1.75 and 1.58 a.u for Sr, Ti and O atoms, respectively. In the LDA approximation, the muffin-tin radii R_{MT} values used are 2.46, 1.87 and 1.61 a.u for Sr, Rh and O atoms for SrZrO₃ compound and 2.5, 1.92 and 1.74 a.u for Sr,Zr and O atoms for SrZrO₃ compound. In SrTiO₃, the R_{MT} values used are 2.44, 1.81 and 1.64 a.u for Sr,Ti,O atoms, respectively. The cut-off energy to separate the core states from valence states is set to be -9 Ry. Inside the sphere, Fourier expanded up to $G_{max}=7$ with a cut-off $l_{max} = 12$ and 35k points in the irreducible Brillion zone with

grid 10 x 10 x10 meshes (equivalent to 1000k points in full Brillion zone) are used to obtain self-consistency for $SrRhO_3$, $SrZrO_3$ and $SrTiO_3$ compounds by GGA.

In LDA, the $G_{max}=8$ with cut-of $l_{max}=14$ and 35k points in the irreducible Brillion zone with grid 10 x 10 x10 meshes.

The Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA) used for the exchange-correlation potential [62], whilemodified Becki-Johnson potential (mBJ-GGA) is used to improve the energy band gap of SrTMO₃[63].

In the (FP-LAPW) method the unit cell is partitioned into two types of regions: (I) atomic centered muffin-tin (MT) spheres with radius R_{α} , and (II) the remaining interstitial region [64].

Chapter Four Result and discussion

4.1 Structural properties

We have optimized the lattice parameters of these compounds by minimizing the total energy. The total energy at different unit cell volumes for $SrTMO_3$ (TM=Rh, Zr,Ti) is shown in Figures4.1,4.2and 4.3.

Figure4.1 shows the fitted total energy versus volume for SrRhO₃by using GGA and LDA approximation, while Figure 4.2 and Figure 4.3 show the fitted total energy versus volume for SrZrO₃and SrTiO₃by using PBE-GGA and LDA methods, respectively.



(a)


Fig.4.1: Equation of state of cubic perovskite of SrRhO₃ (a) PBE-GGA and (b) LDA methods.





Fig.4.2: Equation of state of cubic perovskite of SrZrO₃ (a) PBE-GGA and (b) LDA methods





(b)

Fig.4.3Equation of state of cubic perovskite of SrTiO₃ (a) PBE-GGA and (b) LDA methods

The volume versus energy is fitted by the BrichMurnaghan equation of state [61] to estimate the ground-state properties of these compounds. From this fit, we can get the lattice parameter, bulk modulus and derivative pressure at zero pressure by using PBE-GGA and LDA methods .These values are tabulated in table 4.1, 4.2 and 4.3 for SrRhO₃, SrZrO₃ and SrTiO₃, respectively. In PBE-GGA, the lattice parameters of SrRhO₃, SrZrO3and SrTiO₃ are found to be $3.976 A^{\circ}$, $4.176 A^{\circ}$ and $3.942 A^{\circ}$ respectively. In LDA, the lattice parameters of SrRhO₃, SrZrO₃ and SrTiO₃ are found to be $3.893 A^{\circ}$, $4.103 A^{\circ}$ and $3.865 A^{\circ}$, respectively.

	Lattice parameter(A°)		B _o (Gpa)	B
Method	Present	Others	Present	Present
PBE-GGA	3.976	3.920[65] 4.074[22]	162.550	5.970
LDA	3.893		192.31	4.423
Experimental Results	3.970[65]			

In PBE-GGA, Present results show that the calculated lattice parameter of SrRhO₃ is 0.15% larger than experimental value [65].

In LDA, the calculated lattice parameter of $SrRhO_3$ is 1.97% smaller than the experimental value [65].

. In PBE-GGA, the lattice parameter of $SrRhO_3$ overestimates the other experimental value, while in LDA approximation the lattice parameter underestimates the other experimental value [65].

Table	4.2:	Calculated	lattice	parameter,	bulk	modulus,	pressure
deriva	tive o	f SrZrO ₃ by	using L	DA and PBE	-GGA	methods.	

	Lattice para	ameter(A°)	B _o (Gpa)	B	
Method	Present Others		Present	Present	
GGA	4.176 4.095[65]		150.241	4.241	
	4.177[22]				
LDA	4.103		171.6144	4.456	
Experimental	4.109[66]		150[67]		
Results					

In SrZrO₃, the calculated lattice parameter is 1.6% larger than experimental value [66]. We conclude that present results are to some extent compatible with experimental and theoretical values.

In SrZrO₃, the calculated Bulk modulus is 2.11% larger than experimental value [67].

In $SrTiO_3$, the calculated lattice parameter is 0.9% larger than experimental value [68].

Our results are found to be in good agreement with other experimental and theoretical results [22, 65, 66, 67].

Table	4.3:	calculated	lattice	parameter,	bulk	modulus,	pressure
deriva	tive of	f SrTiO ₃ by	using L	DA and PBE-	GGA	methods	

	Lattice para	ameter(A°)	B _o (Gpa)	B	
Method	Present Others		Present	Present	
PBE-GGA	3.942 3.878[65]		172.25	5.085	
	3.957[22]				
LDA	3.865		201.646	4.085	
Experimental	3.905[68]				
Result					

4.2 Band structure

In this work, we calculate the band structure along the high symmetry line in Brillion-zone of SrTMO₃ (TM=Rh, Zr,Ti) compounds. The Figures 4.4,4.5 and 4.6 show the band structure of SrRhO₃,SrZrO₃ and SrTiO₃ compounds at zero pressure by using PBE-GGA and LDA ,while the Figures 4.7,4.8 and 4.9 show the band structure of SrRhO₃, SrZrO₃ and SrTiO₃ by using mBJ-GGA and mBJ-LDA .Where the Fermi level is set at zero eV.

We tabulated energyband gap results in table 4.4.

Table4.4:	Energy	band	gap(Eg)	of	SrTMO ₃	(TM=Rh,Zr,Ti)
compound	s using LI)A &PE	BE-GGA m	etho	ds.	

Materials	Method	Band gap type	Energy band gap(eV)	Eg-mBJ	Other theoretical results[69]
SrRhO ₃	PBE-GGA		Metallic	Metallic	
	LDA		Metallic	Metallic	
SrZrO ₃	PBE-GGA	Indirect	М→Г3.68	M→Γ4.53	$R \rightarrow \Gamma 3.37$
	LDA	Indirect	М→Г3.455	М→Г4.74	
SrTiO ₃	PBE-GGA	Indirect	М→Г1.954	M→Γ2.748	$R \rightarrow \Gamma 1.92$
	LDA	Indirect	M→Γ1.981	М→Г2.939	





Fig.4.4: Band structure of cubic pervoskite of SrRhO₃ using (a) PBE-GGA and (b)LDA methods.

In PBE-GGA, the valence band maximum (VBM) of $SrZrO_3$ and $SrTiO_3$ occurs along the M-point symmetry line, while conduction band minimum occurs along Γ -point symmetry line with energy gap 3.689 and 1.954eV, respectively.A. Mete *etal.* [69] used peseudopotential method to calculate the values of the energy gap for $SrZrO_3$ and $SrTiO_3$, and found to be 3.37eV for $SrZrO_3$ and 1.92 eV for $SrTiO_3$. These values are found to be in good agreement with our results. In $SrZrO_3$, the calculated energy gap is 8.7% larger than other theoretical value [69].

Thus, SrZrO₃is an indirect wide energy semiconductor and SrTiO₃ is an indirect semiconductor. In SrRhO₃ the energy band gap is metallic. We improved our calculations by using the modified Beke-Johnson potential (mBJ-GGA) [63].

The energy band gapfor SrZrO₃and SrTiO₃ withinmBJ-GGA is still indirect with the same direction as PBE-GGA approach, but it increases by about 0.846 eV and 0.794 eV, respectively. The energy gap of SrZrO₃and SrTiO₃ are 4.535 eVand 2.748eV,respectively by using mBJ-GGA as shown in table 4. SrZrO₃ is an insulator within mBJ-GGA, while it is wide energy band gap within PBE-GGA. On the other hand SrRhO₃has a metallic nature with no energy gap within the two approaches PBE-GGA and mBJ-GGA. SrTiO₃ is semiconductor within two approaches PBE-GGA and mBJ-GGA.



(a)



Fig.4.5:Band structure of cubic pervoskite of $SrZrO_3$ compound using (a) PBE-GGA and (b) LDA methods.



(a)



Fig.4.6:Band structure of cubic pervoskite of $SrTiO_3$ compound using (a) PBE-GGA and (b) LDA methods.

(b)

In LDA , the valence band maximum (VBM) for $SrZrO_3$ and $SrTiO_3$ occurs along the M-point symmetry line, while conduction band minimum occurs along Γ -point symmetry line with energy gap 3.455 and 1.981 eV, respectively. In $SrRhO_3$, the energy band gap is metallic as shown in fig.7 (b). We improved our calculations by using the modified Beke-johnson potential (mBJ-LDA) as shown in Figures 10,11 and12. The energy gap for $SrZrO_3$ and $SrTiO_3$ withinmBJ-LDA is still indirect with the same direction as LDA approach, but it increase by 1.285 eV and 0.958eV, respectively.The energy gap by using mBJ-LDA for $SrZrO_3$ and $SrTiO_3$ are 4.744and 2.939eV, respectively. In $SrRhO_3$, the energy gap is stillmetallic within the two approaches LDA and mBJ-LDA. In PBE-GGA and LDA, we show that the SrZrO₃, SrTiO₃ and SrRhO₃ are wide semiconductor, semiconductor and metallic, respectively .In mBJ-GGA and mBJ- LDA, show that theperovskite structure of SrZrO₃, SrTiO₃ and SrRhO₃compounds are insulator, semiconductor and metallic, respectively.

Comparing LDA and PBE-GGA calculations for the $SrZrO_3$ and $SrTiO_3$ we see that the band structure are nearly similar, except the band gap for PBE-GGA is larger than LDA. In addition, the band structures for $SrRhO_3$ are the same.



(a)



Fig.4.7:Band structure of cubic pervoskiteof SrRhO₃compound using modified Becke-Johnson potential (mBJ) (a) within PBE-GGA and (b) LDA methods.





Fig.4.8:Band structure of cubic pervoskiteof SrZrO₃compound using modified Becke-Johnson potential (mBJ) (a) within PBE-GGA and (b) LDA methods.





Fig.4.9:Band structure of cubic pervoskiteof SrTiO₃compound by using modified Becke-Johnson potential (mBJ) (a) within PBE- GGA and (b) LDA methods.

4.3 Density of state

Density of states (DOS) of a system describes the number of states per interval of energy at each energy level available to be occupied.

In this work, we calculate the calculate the total &partial density of state of SrTMO₃(TM=Rh,Zr,Ti).

By using PBE-GGA, the total and partial density of states for $SrRhO_3$, $SrZrO_3$ and $SrTiO_3$ are shown in Fig. (4.10), Fig (4.12) and Fig. (4.14). In LDA, total & partial density of states are depicted in fig.(4.11), fig.(4.13) and Fig.(4.15) for $SrRhO_3$, $SrZrO_3$ and $SrTiO_3$ respectively.

In Figures 4.10 and 4.11, the valence band of SrRhO₃ originates from O-p and Rh-d states. In the valence band; near to the Fermi level; the bands are

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due to the Rh-d states. In the conduction band, the bands are due to the Sr-d with a small contribution from Rh-d, O-p and O-s states. The valence band is composed of majority O-p and Rh-d states, while the conduction band is mainly contributed by Sr-d state.



(c) (d)

Fig 4.10:Total and partial density of state for (a) $SrRhO_{3}$, (b)Sr , (c) Rh and (d) O of $SrRhO_{3}$ compound by using PBE-GGA method.



Fig.4.11 : Total and partial density of state for (a) $SrRhO_3$, (b)Sr, (c) Rh and (d) O of $SrRhO_3$ compound by using LDA method.

In Figures 4.12&4.13, the valence band for SrZrO₃originates from O-p and small contribution from Zr-d, Zr-p and Sr-d states. In the conduction band, the bands are due to Zr-d and Sr-d states with a small contribution from O-p states. Valence band is composed of majority O-p, while conduction band is mainly dominated by Zr-d and Sr-d states.



Fig. 4.12: Total and partial density of state for (a) $SrZrO_3$, (b)Sr, (c) Zr and (d) O of $SrZrO_3$ compound by using PBE-GGA method.



Fig 4.13:Total and partial density of state for (a) $SrZrO_3$, (b)Sr, (c) Zr and (d) O of $SrZrO_3$ compound by using LDA method.

In figures 4.14&4.15, the valence band for $SrTiO_3$ originates from O-p, and small contribution from Ti-d,Ti- p and Sr-d states. In the conduction band,

the bands are due to Ti-d and Sr-d states and small contribution of O-P states. The valence band is composed of majority O-p and the conduction band is mainly contributed by Ti-d and Sr-d states.



Fig 4.14 : Total and partial density of state for (a) $SrTiO_{3,}(b)Sr$, (c) Ti and (d) O of $SrTiO_{3}$ compound by using PBE-GGA method.



Fig 4.15 : Total and partial density of state for (a) $SrTiO_3$, (b) Sr, (c) Ti and (d) O of $SrTiO_3$ compound by using LDA method.

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4.4 Elastic properties

For the compound to be mechanically stable, the computed elastic constants (C_{11} , C_{12} and C_{44}) must satisfy the Born mechanical stability criteria for cubic structures [70,71].

 $C_{11} > 0$; $C_{44} > 0$; $C_{11} + 2C_{12} > 0$; $C_{11} > B > C_{12}$, where B is the bulk modulus.

Elastic constants are related to fundamental solid state phenomena such as brittleness, ductility, stiffness and the mechanical stability of the material [72].

In the present work, we calculate the elastic constant and their related properties under zero pressure.

Elastic constants are used to estimate other elastic properties such as bulk modulus (B), shear modulus (S), B/S ratio, Young's modulus (Y), Poisson's ratio (v) and anisotropic factor (A). Elastic constants and their related properties of the cubic SrTMO₃ (TM=Rh, Zr,Ti) are listed in table 4.5.

For cubic crystal, the bulk modulus and shear modulus estimated by Voigt and Reuss approximations [73, 74]. The bulk modulus for cubic structure can be given as:

$$B_0 = \frac{1}{3}(C_{11} + 2C_{12})(4.1)$$

Voigt shear modulus S_v and Reuss shear modulus S_R are given by the following two equations:

$$S_{\nu} = \frac{1}{5} (C_{11} - C_{12} + 3C_{44}) (4.2)$$
$$S_{R} = \frac{5c_{44}(c_{11} - c_{12})}{4c_{44} + 3(c_{11} - c_{12})} \quad (4.3)$$

Hill shear modulus S_H is the average value of Voigt shear modulus and Reuss shear modulus:

$$S_H = \frac{1}{2}(S_v + S_R)$$
 (4.4)

Young's modulus (Y) is the ratio of stress to strain, Y gives us more information about the materials stiffness, the greater the value of (Y), the stiffer the material is, Y is given by:

$$Y = \frac{9S_H B}{(S_H + 3B)} \quad (4.5)$$

Poisson's ratio and anisotropic factor can be computed by using bulk and shear modules, Poisson's ratio and anisotropic factor can be given by:

$$\mathbf{v} = \frac{3B - 2S}{2(3B + S)}$$
(4.6)
$$A = \frac{2c_{44}}{c_{11} - c_{12}} (4.7)$$

Elastic constant, Bulk modulus, Shear modulus, young's modulus, Poisson's ratio and anisotropic factor are represented in table 4.5 along with experimental results and theoretical calculation [22.75, 76,77].

Material		C ₁₁	C ₁₂	C ₄₄	В	S	B/S	Y	V	А
SrZrO ₃	Present	319.61	72.543	88.05	154.90	102.2	1.51	251.4	0.23	.7129
	Other theoretical results[75] [22]	338.60 299.16	71.00 72.57	77.00 72.58	160.00 124.76	118.8 74.81	1.34 1.66	 187.04	0.19 0.25	 0.92
SrRhO ₃	Present	239.530	131.168	100.272	167.288	78.324	2.135	203.25	0.29	1.846
	Theory [22]	196.25	99.9	46.28	132.01	47.02	2.80	126.0	0.34	0.97
SrTiO ₃	Present	320.0	97.376	109.68	171.58	110.33	1.55	272.57	0.23	0.985
	Other theoretical result[22], [76]	273.46	85.18	96.90	147.94 200	95.78 109.16	1.54	236.33	0.23	1.02
	Exp.[77] Results				184.00					

 Table 4.5: Calculated elastic constants of SrTMO₃(TM=Rh,Zr) by using GGA

The bulk modulus and shear modulus can be used to measure the material hardness [78], from S values we can see that $SrTiO_3$ is stiffer than $SrZrO_3$ and $SrRhO_3$.

B/S ratio distinguishes the ductility and brittleness of the material, if the value of B/S is greater than 1.75, material behaves in ductile nature; otherwise the material behaves in brittle nature. In present work, the B/S ratio of SrRhO₃,SrZrO₃ and SrTiO₃at zero pressure is 2.135, 1.51and 1.55, respectively. SrRhO₃ has a ductile nature, while SrZrO₃and SrTiO₃ have a brittle nature. On the other hand, one can use Cauchy's pressure to describe the ductility of materials, where the Cauchy's pressure is a difference between C_{12} and $C_{44}(C_{12} - C_{44})$. Pettifor found that if Cauchy's pressure is positive then the compound is ductile otherwise the compound brittle [79], from table 4.5 is easy to see that the Cauchy's pressure is positive for SrRhO₃ compound and negative for SrTiO₃ and SrZrO₃ are brittle, these results are clearly compatible withB/S ratio above.

The value of Poisson's ratio is used to measure the stability of material and give us good information about the nature of bonding forces. If the value of Poison's ratio greater than 0.25, material has ionic bond; otherwise the material has covalent bond. In present work, the Poisson's ratio of SrRhO₃, SrZrO₃ and SrTiO₃ are 0.29, 0.229 and 0.23, respectively. SrRhO₃ has an ionic bond, while SrZrO₃ and SrTiO₃have a covalent bond.

The anisotropy factor is an important parameter to measure of the degree of materials anisotropy; also it has a significant usagein engineering scienceto inspect the potential of micro-cracks in the material [80,81]. The value of anisotropy factor is unity for completely isotropic material, otherwise material is elastic anisotropy. In present work, A of SrRhO₃, SrZrO₃ and SrTiO₃ 1.846, 0.7129 are and 0.985, respectively. SrRhO₃, SrZrO₃compounds are anisotropic compounds, while SrTiO₃ compound is isotropic .A for both deviates from unity, SrRhO₃ has a large elastic anisotropy, while SrZrO₃ and SrTiO₃ have a small elastic anisotropy. If we compare present estimated elastic constants of SrRhO₃, SrZrO₃ and SrTiO₃ with experimental and theoretical results, we can conclude that, present results in a good agreement with experimental and theoretical result with small deviations [22,75,76,77]. We claim that our result are accurate than other theoretical values because we use all electron method[22].

4.5Optical properties

The optical properties of material are important to understand the electronic structure and other physical properties. In present work, we investigate the dielectric constant and other optical parameters of SrTMO₃ (TM=Rh, Zr,Ti). These optical parameters are depicted in Figures 4.16-4.20.

Optical properties of these compounds are obtained from the frequency dependent complex dielectric function $\varepsilon(w)$, which is given by the Ehrenreich and Cohen's equation [82.].

$$\varepsilon(\mathbf{w}) = \varepsilon_1(\mathbf{w}) + i\varepsilon_2(\mathbf{w}) \tag{4.8}$$

Dielectric function $\varepsilon(w)$ equation 4.8, has two parts, real part $\varepsilon_1(w)$ and imaginary part $\varepsilon_2(w)$.Real part is related to the polarization of the charge inside the solid, while imaginary part describes the absorption behavior. The dielectric constant is needed to compute other optical properties, such as refractive indexn(w), reflectivity R(w), extinction coefficient k(w), energy loss function L(w) and absorption coefficient $\alpha(w)$ which can be written as [83,84.85]:

$$n(w) = \left(\frac{1}{2} \left[\sqrt{\epsilon_1^2(w) + \epsilon_2^2(w)} + \epsilon_1(w) \right] \right)^{1/2}$$
(4.9)

$$R(w) = \left|\frac{\sqrt{\varepsilon(w)} - 1}{\sqrt{\varepsilon(w)} + 1}\right|^2 = \left|\frac{\sqrt{\varepsilon_1 + i\varepsilon_2} - 1}{\sqrt{\varepsilon_1 + i\varepsilon_2} + 1}\right|^2$$
(4.10)

$$k(w) = \left(\frac{1}{2} \left[\sqrt{\epsilon_1^2(w) + \epsilon_2^2(w)} - \epsilon_1(w) \right] \right)^{1/2}$$
(4.11)

$$L(w) = \frac{\varepsilon_2(w)}{\varepsilon_1(w)^2 + \varepsilon_2(w)^2}$$
(4.12)

$$\alpha(w) = \frac{\sqrt{2}w}{c} \left(\sqrt{\epsilon_1^2(w) + \epsilon_2^2(w)} - \epsilon_1(w) \right)^{1/2}$$
(4.13)

In Figure 4.16 (a) and (b) and Figure 4.19 (a), the real and imaginary parts of dielectric function are illustrated forSrRhO₃, SrZrO₃and SrTiO₃, respectively as a function of photon energy in the range from 0 to 14 eV. It can be seen from the Figure 4.16(a) and (b) and Figure 4.19that $\varepsilon_2(w)$ is starting to have a considerable value from 0.3 eV for SrRhO₃, while $\varepsilon_2(w)$ of SrZrO₃ and SrTiO₃ starts from about 3.6, 2eV, respectively. After threshold energy, we observed some peaks; these peaks originate from electrons transitions from valence band to conduction band. Threshold energies of SrRhO₃, SrZrO₃and SrTiO₃ are 0.3 eV, 4 eV and 2.2, respectively. The real part $\varepsilon_1(w)(\varepsilon$ gives us information about the polarizability f a material, the static dielectric constant $\varepsilon_1(w)$ of SrRhO₃, SrZrO₃and SrTiO₃ are 11, 3.8 and 5.5, respectively. SrRhO₃ has greater dielectric constant than SrZrO₃and SrTiO₃; metal with high dielectric constant is used for manufacturing high capacitors [86]. The negative values of real dielectric constant; which can be seen in both visible and ultraviolet spectrums of SrRhO₃ and only in the ultraviolet spectrum for SrZrO₃and SrTiO₃; show a metallic behavior of these compounds in the mentioned regions.

In Figure 4.16 (c) and (d) and Figure 4.19 (b), the real and imaginary parts of conductivity are illustrated for SrRhO₃, SrZrO₃ and SrTiO₃, respectively. It can be seen from these figures that the imaginary parts of conductivity are starting to have a considerable values from zero eV, on the other hand the real parts of conductivity for SrRhO₃, SrZrO₃ and SrTiO₃ start to have a considerable value at 0.3 eV, 4 eV and 2.2 eV, respectively. We have also observed some peaks in the conductivity spectra of the studied compounds. The conductivity increases as the material becomes more photons (energy) absorbent.





(b)





(d)

Figure 4.16: The real and imaginary parts of dielectric function of (a) $SrRhO_3$, (b) $SrZrO_3$ compounds and the real and imaginary parts of conductivity of (c) $SrRhO_3$, (d) $SrZrO_3$ compounds.

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(b)



Figure 4.17: The refractive index and extinct factor of (a) SrRhO₃ (b) SrZrO₃ and reflectivity of (c) SrRhO₃ (d) SrZrO₃compoud.

The refractive index and extinct factor are illustrated in Figure 4.17(a) & (b) and Figure 4.20 (a) for SrRhO₃, SrZrO₃ and SrTiO₃, respectively. Extinction coefficient depends on the amount of absorption of photon when propagates in the material, while the refractive index indicates the phase velocity of electromagnetic wave.

In Figure 4.17 (a) & (b) and Figure 4.20 (a), we observe that the extinction coefficients of SrRhO₃, SrZrO₃ and SrTiO₃, start to have considerable values at 0.3, 4 and 2 eV, respectively with some peaks along the spectrum. These peaks are related to the electrons transitions from valence to conduction bands, also it is clear that extinction coefficient and the imaginary part of epsilon vary in the same way. The static value of refractive index n(0) for SrRhO₃, SrZrO₃ and SrTiO₃ are 3.4, 1.9 and 2.3, respectively.

The reflectivity's spectra of SrRhO₃, SrZrO₃ and SrTiO₃as a function of energy are shown in Figure4.17 (c) & (d) and Figure 4.19 (c). The static reflectivity of SrRhO₃,SrZrO₃ and SrTiO₃ are 0 .3, 0 .1and 0.15, respectively, static reflectivity of SrRhO₃ are three times greater than reflectivity of SrZrO₃. The reflectivity value increased rapidly in the high energy region; far ultraviolet region (FUV); for SrRhO₃,SrZrO₃ and SrTiO₃compounds, all compounds are suitable as wave reflectance compounds in the (FUV) region, but unsuitable as transparent compounds.







(b)



Figure 4.18: Absorption coefficient of (a) SrRhO₃, (b) SrZrO₃ and Energy loss function of (c) SrRhO₃, (d) SrZrO₃ compounds.

The absorption coefficient spectra of SrTMO₃ (TM=Rh, Zr,Ti) are plotted in Figure 4.18 (a) & (b) and Figure 4.19 (d). The absorption spectra of SrRhO₃, SrZrO₃and SrTiO₃ begin at about 0.8 eV, 3.8 and 2eV, respectively. The observed peaks in the spectra related to electrons transitions from valence toconduction bands. These two compounds are good absorbent compounds, but not in the low and FUV regions.

The energy loss function $L(\omega)$ is describing the energy loss of the fast electrons propagates inside the material. The energy loss spectra of SrRhO₃, SrZrO₃and SrTiO₃are depicted in Figure 21 (c) & (d) and 23 (b). We observe some peaks, the highest peaks related to the plasma frequency [87]. From figures the plasma frequency of SrRhO₃, SrZrO₃ and SrTiO₃ occur at 12, 13 and 11eV, respectively.





(b)


Figure 4.19: The real and imaginary parts of dielectric function of (a) $SrTiO_3$, (b) the real and imaginary parts of conductivity, (c) the refractive index and extinct factor, (d) and the reflectivity.



(a)



Figure 4.20: The refractive index and extinct factor, of (a)SrTiO₃ (b) and the loss energy.

Chapter 5 Conclusions

The lattice parameter is calculated to be in good agreement with experimental and other theoretical results. The band structure shows that the SrRhO₃ has a metallic behavior within both PBE-GGA and mBJ-GGA approaches, while SrTiO₃ shows a semiconductor behavior in LDA and GGA approximation. SrZrO₃ shows a wide semiconducting behavior in GGA and LDA approximation and it shows an insulating behavior using mBJ-GGA method. The elastic constant (C_{11}, C_{12}, C_{44}) , bulk modulus, shearmodulus and young' modulus are also calculated and discussed. By analyzing B/S ratio and Poisson' ratio, we find that SrRhO₃ has ductile nature, while SrZrO₃ and SrTiO₃have brittle nature. SrRhO₃ has ionic bond While SrZrO₃ and SrTiO₃ have covalent bond. The optical properties such dielectric constant, absorptioncoefficient, reflectivity coefficient, as refractive index, optical conductivity and energyloss function were investigated in the energy range (0-14) eV. According to the dielectric constant, SrRhO₃ has greater dielectric constant than SrZrO₃ and SrTiO₃. In conclusion, our elastic calculations for SrTiO₃ are compared with experiment and theoretical results and found to be in good agreement. Our calculations for SrTMO₃ (TM=Rh, Zr,Ti) will help to use these compounds for practical applications.

Lattice	SrRhO ₃	SrZrO ₃	SrTiO ₃
parameter			
present	3.976	4.176	3.943
Exp.[65]	3.970 [4.109	3.905
Theoretical	4.074	4.177	3.957
[22]			

Our results for the lattice parameters are summarized in table 5.1 and compared with other experimental and theoretical results. Our results are more closed to the experimental results than other theoretical results.

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جامعة النجاح الوطنية كلية الدراسات العليا

الخصائص التركيبية والالكترونية والمرونيةوالضوئية لمركبات SrTiO3وSrZrO3 وSrRhO: دراسة الجهد التام المزيد ذو الموجات المستوية الخطية

إعداد

أريج معروف عبد اللطيف شواهنه

إشراف

د.محمد سلامة أبو جعفر

قدمت هذه الإطروحة استكمالاً لمتطلبات الحصول على درجة الماجستير في الفيزياء، بكلية الدرسات العليا، في جامعة النجاح الوطنية، نابلس – فلسطين.

الخصائص التركيبية والالكترونية والمرونية والضوئيه لمركبات SrZrO3 وSrZrO3 وSrZrO3 دراسة الجهد التام المزيد ذو الموجات المستوية الخطية إعداد أريج معروف عبد اللطيف شواهنه أريج محمو سلامة أبو جعفر الملخص

تم فحص الخصائص الضوئية والمرونية والإلكترونية والتركيبة لمركبات البيرفيسكايت المكعب TM=Ti, Zr, Rh)SrTMO₃)عن طريق استخدام الجهد التام المزيّد ذو الموجات المستوية PBE-GGAواستخدام تقريب الكثافةالمحليةLDAوالتقريب التدرجي المعممPBE-GGA ضمن إطار نظرية الكثافة الوظيفية (DFT).

لتحسسين فجوة الطاقة للمركبات تم استخدام نظام بيكي جونسون المعدلmBJحيث تم ايجاد الخصائص التركيبية مثل(ثابت الشبكةالبلورية ومعامل الحجم والمشتقة الاولى للضغط) وكانت متوافقة مع النتائج النظرية والتجريبية الاخرى.

- من اهم النتائج في هذه الدراسة:
- 1- النتائج والحسابات الحالية توافقت وبشكل جيد مع النتائج النظرية والنتائج التجريبية.
- 2- تبين ان المركبSrRhO3معدني السلوك وتبين ان المركب SrZrO3هو مركب عازل وتبين
 ان المركبSrTiO3هو مركب شبه موصل.
- 5- وُجد ان مركب SrRhO3 قابل للسحب والطرق بينما تم اعتبار المركبين SrZrO3هر SrTiO3مركبات هشَة الانكسار.
- 4- يمتلك المركب SrRhO3 روابط ايوينة بينما يمتلك المركبين الاخرين SrZrO3 دSrTiO3روابط تساهمية.
- 5- يمتلك المركب SrRhO3 ثابت عازليه للتيار الكهربائي اكبر من المركبين الاخرين SrZrO3و SrTiO3.