Ab-Initio Study of Electronic and Structural Properties for BaSnO₃ Compound Using DFT Calculations and FP-LAPW Technique in Wein2k Software

Zubair Ashraf (✉ zubair@stu.pku.edu.cn)

Peking University <https://orcid.org/0000-0002-6909-5795>

Daud Rafique

University of the Punjab Quaid-i-Azam Campus: University of the Punjab

Tahir Mehmood

University of the Punjab Quaid-i-Azam Campus: University of the Punjab

Daniyal Akbar

University of the Punjab Quaid-i-Azam Campus: University of the Punjab

Research Article

Keywords: PPV(Perovskites photovoltaic), SP(Structural Properties), EP (Electronic Properties) DFT (Density Functional Theory)

Posted Date: March 24th, 2021

DOI: <https://doi.org/10.21203/rs.3.rs-325590/v1>

License: © ⓘ This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

Zubair Ashraf ^{a*}, Mphil Physics, Ph.d Material Science

Daud Rafique ^b Mphil Physics ,

Tahir Mehmood ^b Mphil Physics

Danial Akbar ^b Mphil Physic, Ph.d

^{a*} Department of Materials Science and Engineering, Department of Energy and Resources
Engineering College of Engineering, Peking University

^b Department of the Physics, University of the Punjab Lahore, Pakistan.

Abstract

(Perovskites Photovoltaic) PPV cells are the hottest topics in solar cells in the recent years, because of the remarkable structural and electronic properties and hence rapid progress in material science. The Challenge associated with high-mobility BaSnO₃ films is to grow. It shows high carrier mobility and UV-visible transparency has been attracting more and more attention as a very promising component for the next generation opto-electronics. Here, we demonstrate a Structural and Electronics properties (Sp and Ep), To characterize this compound theoretical calculation have been performed by using first principal method and the results show BaSnO₃ is conductor at 0eV i.e. room temperature and gaining energy make more conduction transferring more electrons from conduction to valence bands. BaSnO₃ shows 5.78e.v maximum for the conduction. We have studied this compound in ideal cubic phase. At 0° Kelvin calculation are performed to get different properties. No experimental studies have been done on this compound. And it was difficult to accumulate its experimental data. WC-GGA is used for the study of structural properties of BaSnO₃. This Correlation potential can also be used for the calculation of the various perovskite. Depending on the cubic (ABX₃) composition, perovskites exhibit a wide range of structural and electronic properties, which are optimized for different applications.

Keywords: PPV(Perovskites photovoltaic), SP(Structural Properties), EP (Electronic Properties) DFT (Density Functional Theory)

Corresponding Author: Zubair Ashraf (+923082528918)
Email: Zubair@stu.pku.edu.cn

Contents

1.0 Introduction	3
1.1 Stability Conditions of All Perovskites	4
1.2 My Perovskites Compounds	5
1.3 Individual Element	5
1.4 Some Parameters, Ba, Sn, and O	7
1.5 Tolerance Factor.....	8
1.6 Some Applications of Perovskites	9
2.1 Introduction to Density Functional Theory	9
2.1 Execution of DFT.....	10
2.2 Boundaries of DFT	11
3.0 WIEN2k Software	11
3.1 Introduction to Wien2k.....	11
3.2 Compatibility	12
3.3 Working.....	12
3.4 Wien2k Application.....	12

Corresponding Author: Zubair Ashraf (+923082528918)
Email: Zubair@stu.pku.edu.cn

3.5 Software codes	13
3.6 Structure Generation	13
3.7 View Structure.....	13
3.8 Initialize the Calculation.....	13
3.9 Volume Optimization Curve	14
3.10 Evaluation of Properties	15
4. Results and Discussion	15
4.1 General Behavior of BaSnO ₃	15
4.2 Structural Properties of BaSnO ₃	15
4.3 Structure View of the BaSnO	17
4.4 Optimization Curve BaSnO ₃	17
4.5 Electronic Properties.....	18
5.0 References:	21

1.0 Introduction

High-mobility of the perovskite BaSnO₃ films are of significant interest as new wide band-gap semi-conductors for the power electron as a new transparent conducting oxide and as a wide bandgap semiconductor for power electronics. To characterize this compound theoretical calculation have been performed by using first principal method and the results show BaSnO₃ is conductor at 0eV i.e. Perovskites belongs to oxide family which has studied yet. They show many important and interesting most properties. Perovskites exhibit polarization if we apply electric field. The basic purposes of this thesis are “The first

Corresponding Author: Zubair Ashraf (+923082528918)
Email: Zubair@stu.pku.edu.cn

principal study of electronic properties for BaSnO_3 compound using DFT calculations in wein2k code”. According to the best of my knowledge this work has been done for the very first time.[1]

1.1 Stability Conditions of All Perovskites

The conditions required for a stable perovskite is:

- i. Valance bond should be balanced.
- ii. Ionic radii must fulfill the condition of Goldschmidt’s criteria

Goldschmidt perform great work on the study of perovskites, He determine the tolerance factor for perovskites. [1, 2]

Figure (1.1): The basic cubic structure of Perovskites.

These compounds are stable in nature perovskite general structure is cubic but in actual it occurs at pseudo cubic [3]. at the corner there is atom A and at the center there is atom B and Atom X is at the face center of cube.

Table (1.1): Occupation of atoms in simple perovskites.

Atoms	Coordinates
-------	-------------

A Cation	(0,0,0)
B cation	(1/2 ,1/2 ,1/2 ,)
X anion	(1/2 ; 1/2, 0), (1/2 , 0,1/2) (0,1/2,1/2,)[4]

1.2 My Perovskites Compounds

By using general formula of ABX_3 , My perovskites compound on which my searching is continuous, is Barium Tin Oxide or also known as Barium titanite.

1.2.1 BaSnO₃

It is a semiconducting oxide with wide band gap of 3.1 eV. Recently, it is discovered that BaSnO₃ doped with few percent of Lanthanum exhibits unusually high electrical mobility[5], at room temperature and superior thermal stability at high temperatures [6].

It has a very low dielectric response (range from 4.9-6.6). This oxide is stable against zone center phonons in cubic perovskite structure as well as KTaO₃ and BaZrO₃ also same oxides as Barium tin oxides.

1.3 Individual Element

1.3.1 Barium (Ba)

It was found by S.H. Davy in England in 1808. It is named after Greek word “Barys” which means heavy. Symbolically it is represented by *Ba*. It is s-block element and a member of period 6 with atomic number 56. It is fifth element of group two. It is alkaline earth metal which is very reactive. It is metallic element which exist is soft solid and it is silvery white like lead in pure form. It is good electrical conductor. [7]

It easily reacts with water and alcohol. In glasses and paints small proportions of barium elements are added. Barium in salt form also used in flames to change the color to green. It has body centered cube crystal structure[7].

Figure (1.3.1): An Ore of Barium

1.3.2 Tin (Sn)

General symbol for the Tin is (Sn). It is not present in earth in free element form. The most famous ore for the Tin is Cassiterite that is Tin Oxide SnO_2 . It is anglo-Saxon word which is derived from Latin “Stannum” means Tin. It has Atomic number is 50. Electronic configuration is $(\text{Kr}) 4d^{10} 5s^2 5p^2$.

In ancient times conversion of other metal into gold was done by Tin which is known as Alchemy[6, 8]. Its crystal structure is existing into two forms that is cubic and tetragonal known as alpha-tin and beta-tin. It is used in marine environments because it is fungicide and bactericide. Usually it is silvery white metal with highly crystalline structure.

Figure (1.3.2): An ore of Tin

It is p-block element in fifth period of periodic table. It is metallic element of fourth member of group 14 [9].

1.3.3 Oxygen (O)

Most important part of our life. It is chemical element having atomic number 8 and mass number 15.999. it is denoted by (O). It is found in non-metal group. It is oxidizing agent and second most electronegative element in periodic table[8]. It is third most plentiful gas on our planet after hydrogen. It is colorless, odorless in gaseous form, but in liquid or solid form it is blue in color. It was named by Antoin lovoiseir in 1977[8, 9].

Figure (1.3.2): Oxygen in liquid form

1.4 Some Parameters, Ba, Sn, and O

The values of different parameters related with different assets are given as :

Table (1.2): Some important parameters of Ba, Sn, and Oxygen.

Characteristic	Barium	Tin	Oxygen
Symbol	Ba	Sn	O
Atomic No,	56	50	8
Group	2	5	16
Period	6	5	2
Density(g/cc)	3.51	7.30	1.42
Melting Point	725° C	231.97° C	-219° C
Boiling Point	1897° C	2602° C	-183° C
Covalent Radius (Å)	1.98	1.41	66

Corresponding Author: Zubair Ashraf (+923082528918)
Email: Zubair@stu.pku.edu.cn

Oxidization State	+2	+4.2	-2
<u>Specific Heat</u>	0.204 (J/gk)	0.227 (J/gk)	0.130 (J/gk)
Lattice structure	Body-center cube	Tetragonal	Monoclinic at solid
Appearance	soft, silver-white metal	silvery-white, soft, <u>ductile-metal</u>	Liquid, and solid oxygen Is pale blue [9, 10]

1.5 Tolerance Factor

It was determined in 1926 by Victor. M Goldschmidt. Tolerance factor was introduced to measure the distortion in perovskites from their ideal cubic structure. There is great importance of Cationic and Anionic radii of atoms in perovskite compound which plays an important role in the alteration of ideal cubic structure[11]. The deviation of orthogonal, rhombohedral can be determined by using of G. schmidt tolerance factor is given as:

$$t = r_A + r_X / \sqrt{2} (r_B + r_X) \quad (1.1)$$

where r_A and r_B are the ionic radii of the cations and r_X is the ionic radii of anion[12]. For the ideal cubic perovskites values of the tolerance factor should be equal to 1. But in the case of the distorted perovskites that value changed from 1. Equation 1.1 describes that sum of ionic radii is nearly equal to the bond length[13]. Tolerance factor for the different structure is shown in table 1.3.

Table (1.3): *The values of tolerance factor for different structure.*

Tolerance Factor	Structure	Ionic Radii	Example
> 1	Hexagonal	A and B both are so small	BaNiO3

0.9 to 1	Cubic	A and B have ideal size	SrTiO₃
0.71 to 0.9	Orthorhombic	A is so small than B	CaTiO₃
< 0.71	Trigonal or Different structure	A and B both have similar Radii	FeTiO₃[14, 15]

1.6 Some Applications of Perovskites

Due to some remarkable physical, chemical and structural properties, they have an important place in the world of science research. These multi purposes causes many applications of the perovskites and thus have an important place in the Industry field. A perovskites oxide Barium titrate have so much variety of applications because of ionic and mixed conductivity it is used as capacitors, thermistors, temperature co-efficient, and piezoelectric devices (in which device produces AC voltage when we apply mechanical stress) etc [[13](#)]. perovskites that are used in highly effective photovoltaic are synthetic perovskites[[15](#)]. They are prepared same as solar cell by method of thin film[[14](#)]. They are also used to produced Laser light, when LiAlO₃ is doped with neoydium they produce laser light of 1080nm. Those perovskites have high resistivity are used in dielectric material, some of them are LaTiO₃, LaVO₃, etc. and some of them are good conductor because B atom in ABO₃ having oxidization state of +2[[16](#)]. They are also used in oxygen sensor like SrTiO₃.

2.0 Introduction to Density Functional Theory

To understand the internal forces of the atoms when they join in the solids and to study the different properties (like thermal, electronic, magnetic and optical, etc.) of the solids, different theories were postulated with the passage of time. Nowadays the most acceptable theory in regard with the measurement of the different properties of matter or solids is “Density Functional Theory” . It was developed by W. Kohn and J. Pople. Walter Kohn was awarded by the Noble Prize in 1998 for the development of DFT.

This theory was developed by the combination of the two theorems which was given in the 1960’s [[17](#), [18](#)]by:

- Hohenberg-Kohn in 1964.
- Kohn-Sham in 1965.

A simple glance on the background in table is given as:

Table (2.1): Development of DFT from beginning.

Year	Work
1920s	Introduction of Thomas fermi model.
1964s	Hohenberg-Kohn proves existence of DFT.
1965s	Kohn-Sham scheme introduction.
1970s to early 80s	LDA, DFT becomes useful.
1985s	Incorporation of DFT into molecular dynamics.
1998s	Noble prize awarded to Walter Kohn in Chemistry for work in DFT. [18, 19]

2.1 Execution of DFT

In an external potential of atomic nuclei Density Functional Theory is the most successful theory of today science and used for the study of the properties of system of electrons. The major advantage of the Density Functional Theory is reduction $3N$ degree of freedom of a system to three degree of freedom that made Density Functional Theory able to solve complicated system[20]. It gives ground state properties of material which further used to understand the behavior of that material with other materials, in general it gives the theoretical approach to the physical properties as well as electronic, optical, thermal, magnetic and electrostatic properties on the ground state level[21]. In respect to the Chemistry approach Density Functional Theory is also a successful theory, in which it has many applications.

It is used to measure the following bonds:

- Bond length.
- Bond angles.
- Nature of Bonds[22]. It has importance in the biological field, material like nanotubes, proteins, and carbon. Optimization as well as atomization energies are also measurable because of Density Functional Theory. Density Functional Theory has direct relation of ground state energy of the system with its electron density. This electron density is actually main variable on which whole Density Functional Theory exists[21, 22].

2.2 Boundaries of DFT

DFT cannot be useful to determine each and every properties and has deficiencies in determining some properties listed below:

- Band Gap

Absolute values of band gap cannot be determine.

- Superconductivity

Accurate prediction is not available in DFT.

- High temperature properties.

Unable to calculate the properties at higher temperature close to melting points[19, 21, 22].

3.0 WIEN2k Software

3.1 Introduction to Wien2k

To calculate electronic, structural, magnetic, thermal, optical and many others properties of the materials in SSP in which we use the concepts of density functional theory these all can be measured in single package called Wien2k software. One of the most and accurate methods of full potential is linearized augmented plane wave method (LAPW), which is used to calculate band structures and it is the base of the wien2k package. Wien2k deals with the electrons and their relativistic effects and many others features like quantum mechanical properties.

Fig 3.1

The first copyright version was Wien, it is introduced by Peter Blaha, George Madsen, K.H Schwarz, and D. Kvasnicka[1]. 2000+ groups have the license which shows the importance. Many precise and updated version of the UNIX have been developed which were Wien93, Wien95, and Wien97. Today the most updated version of the Wien2k is Wien2k_18.2[1].

3.2 Compatibility

Wien2k is a computer program having FORTRAN90 language, which require UNIX operating system, and the installation in which program are connected through C-Shell script.

Following are the computers systems on which Wien2k can be run successfully.

- IBM RS6000
- Intel Pentium PC, s working Under LINUX
- HP
- SUN
- DEC Alpha
- SGI

Hardware requirement are different for the different cases for example having 10 atoms per unit cell run on the Pentium-II PC with memory 128 MB under LINUX. But for the powerful PC disk space up too few GB is recommended.

But the demand for the software is 1 GB disk space and 512 MB cache memory.

3.3 Working

We are dealing our compounds in ideal conditions in material science and in ideal crystals. We consider the crystal at 0°k temperature, thus we can calculate many properties at ground state level. Like every software we use exchange correlation potential in Wien2k also [1, 23, 24].

3.4 Wien2k Application

To understand the structure and many properties of an atom or compound it has many applications in the field of Science.

- ✓ It is used to solve Kohn-Sham Equation of DFT.
- ✓ For the calculation of structural properties.

- ✓ It is computational program which is used to study the ideal compound.
- ✓ It is used to calculate electronic properties, density of the states, and band structure.
- ✓ Optical, elastic and magnetic properties are measured through Wien2k software.
- ✓ It is used for the calculation of the electron energy loss spectrum, core loss spectrum [25].

It determines the elastic constants for cubic cases.

3.5 Software codes

It consists of many independent FORTRAN90 programs, which are linked to each other's through C-shell script. This software can be executed using any web browser or w2web interface. We used wien2k software by using short commands. The main steps for the software are;

- Define structure.
- Initialize all commands.
- SCF (run self-consistent-field

These are the basic building block for the run to this software[26].

3.6 Structure Generation

First, we need to generate structure of the compound to find out the properties of the compound. We need to click on the struct-gen command and then put all the values of the compound like position of each atom, number of atoms, lattice constant, angels of atoms, and space group. By entering all commands, we have to click on Save structure, after that RMT is automatically set, by continuing editing structure file is saved[3].

3.7 View Structure

After input all data of the given compound and executing then click on the View_struct to view the structure of the compound.

3.8 Initialize the Calculation

After saving the structure, now we are going to initialize the calculations for properties with symmetry. Init_lapw term is used to initialize the command, initialization depends upon the 6 properties, these properties perform different task.

These are given as:

❖ **X-nn**

In this term ‘nn’ stands for nearest neighbor distance, this is used to calculate the distance between spheres and for checking the overlapping of all atomic spheres.

❖ **X-sgroup**

It specifies the space group and point group of the non-equivalent atoms. It can also distinguish the different atoms by using value of the Z uniquely. It can find out the smallest unit cell and also shift the origin of a unit cell.

❖ **X-symmetry**

Space group symmetry is checked by the ‘X-symmetry’ command. This program gives the atomic densities of the compound.

❖ **X-lstart**

It is also called LSDA programing it is start by Hartree units at input and end on Rydberg units at output. This program can also produce atomic potential.

❖ **X-kgen**

This produce k-mesh by converging all the k points in an irreducible region of the brillouin zone.

❖ **X-dstart**

To make initial density of crystalline solids calculation from x-lstart is superimposed. This program is called “superposition of the Atomic Density”.[27]

3.9 Volume Optimization Curve

To find out shape and size of the unit cell having total energy optimization process is used. Shape and size are very important parameters. We use experimental values as a input, to calculate the total energy of the perovskites compound this can be measured by the use of Murnaghan Equation.

$$E(v) = E_0(v) + BV / B' (B' - 1) [B \{ 1 - V_0 / V \} + (V_0 / v) B' - 1] \quad (3.1)$$

In equation (3.1) we have:

$E_0(v)$ = Ground state energy

V = ground state volume.

B = bulk modulus.

B' = bulk modulus pressure.

E(v) energy verses volume Curve.

(3.1) equation is the second order equation which gives the ground state energy and volume. Thus, we can calculate energy by entering the values of volume[28]. Therefore, its graph is always parabola along y-axis. The graph is plotted between V and E. This process is known as Volume optimization, the lattice constant is also determined from the equilibrium volume. The range of the graph tells us how much time is required to give volume optimization[29].

3.10 Evaluation of Properties

After SCF cycle, the properties of the given compound is obtained and calculated, like, electronic, optical, etc. can be obtained using wien2k software. since, we know the properties of the material or compound, we can use these into the field of science[30].

4. Results and Discussion

4.1 General Behavior of BaSnO₃

In order to characterize this compound theoretical calculation have been performed by using first principle method. I have studied this compound in ideal cubic phase. At 0° Kelvin calculation are performed in order to get different properties. No experimental studies have been done on this compound. And it was difficult to accumulate its experimental data.

BaSnO₃ having space group 221_{pm}3m. Barium Stannate (BaSnO₃) depending on temperature it have different types of structures. It shows many dramatic properties for example ionic conductivity, superconductivity, colossal magnetoresistance[30-32], as well as ferromagnetism and ferroelectricity and semi-conductivity⁷⁰. It also shows piezoelectric and optical properties which have great importance in microelectronics and telecommunications respectively[21, 32].

In this chapter I will study structural and electrical properties of BaSnO₃ along with graphs in WEIN2k software.

4.2 Structural Properties of BaSnO₃.

WC-GGA is used for the study of structural properties of both BaSnO₃. This Correlation potential can also be used for the calculation of the various perovskites. It is comparatively

most accurate technique having less uncertainty. For the very first compound the orientation is adjusted in such a way that Ba is placed at origin and location of Atom in compound is (0,0,0), and for Sn it is in the center of the cubic structure with location (1/2,1/2,1/2), and for the last atom oxygen is in the face centered having location (1/2,1/2,0), (1/2,0,1/2), and (0,1/2,1/2). For the structural properties of BaSnO₃ it needs input parameters like, lattice constant, space group, and atomic positions of the every atom etc. These parameters are given as below in table.

Table 4.1 Input Parameters for Structural Properties

BaSnO₃		
Parameters	Names	Values
Angles	A	90°
	β	90°
	γ	90°
Atomic Number (Z)	Ba	56
	Sn	50
	O	8
Position	Ba	(0,0,0), (1/2,1/2,1/2),
	Sn	{(1/2,1/2,0),(1/2,0,1/2),
	O	(0,1/2,1/2)}.
Lattice Constant	A	4.189 Å
	B	4.189 Å
	C	4.189 Å
Space Group	221	Pm-3m
Potential	Exchange correlation	WC-GGA
RMT	Ba	2.50 Å
	Sn	1.97 Å
	O	1.70 Å

4.3 Structure View of the BaSnO

I have performed all steps as mentioned above, for the calculation of the structural properties required. Steps are done one by one to calculate the structural properties. By using WEIN2k package structure of the BaSnO₃ can be obtained which is given in below figure (4.1). In this structure 'Ba' is at the corner of the cube and 'Sn' is in the center of the cube, and 'O' is at the face centered position.

Figure 4.1 ideal cubic unit cell of BaSnO₃

4.4 Optimization Curve BaSnO3

In case of BaSnO₃, the increase in volume of the unit the values of the energy decreases of the crystal structure. The certain value of the volume which is minimum energy of the volume, after this value energy of the volume increases, this is called optimized equilibrium energy, because the system is in the equilibrium.

The Energy-Volume curve for this compound is plotted in given figure, The value of the GSE and V for BaSnO₃ is obtained 29088.815 Ry and 494 (a.u)³ respectively. Some other important parameters of the BaSnO₃ can also be obtained like,

Figure 4.3 The total energies of the cell volume of BaSnO₃

pressure derivatives of the bulk modulus and Bulk modulus at 0 value[21, 22, 33]. Bulk Modulus is the ability to stand against compression with its original unit volume, and its

shape is also retainable, up to the value of pressure which is applied. It can also be obtained as:

$$B = \frac{\text{Stress}}{\text{Strain}}$$

All these properties are calculated by Wu Cohen-GGA Approximation using Wien2k package.

4.5 Electronic Properties

Those properties which are related to the electrons are called electronic properties, which gives the behavior of the electrons within the crystal. Some of the useful result that I have determined about electrons are:

- ✚ Density of the States
- ✚ Band Gap
- ✚ Electrons Density

Each of them is explained as:

4.5.1 Density of states

It can be defined as “Energy levels available to be occupied by electrons per unit energy range”. Mathematically it is given as:

$$D(E) = \frac{d\Omega(E)}{dE}$$

Whereas $d\Omega$ represents the no. of the states, these states can be written as:

$$D(E) = \sum \int (d^3 k \times \delta(E - \epsilon_n(k))) / (2\pi)^3 \quad 4.3$$

ϵ_n is eigen value energy[34] I have drawn the graph of the density of the states, with the help of Wien2k software,

This graph are plotted between energy and DOS.

The unit used for the energy is eV and for the DoS is (states/eV), the energy is taken along the x-axis and DoS is on the y-axis. This graph show increase and decrease in the energy and DOS.

Five atoms combine to make the unit cell of each of my compound (BaSnO_3). Each atom shows

different configuration and valence electrons as well as conduction states, every peak

Figure 4.5 Total density of states for BaSnO₃

In the Graph shows different orbitals[28]. Valence electrons are nearly very close to the conduction's electrons, when they jump from one band to another attain some energy as photons, and hence peaks show only for the valence electrons in the DOS.

4.5.2 Electrons Density

The measure of the probability of the electrons around the atom is called electron density, which gives the bonding between atoms[32]. ED has relation with wavefunction of the electrons. Electron density gives the information about bond nature and about interaction between atoms.

For finding electron density of my compounds I have used 2-D plots for the electron density,

The electrons density for the perovskite's compounds BaSnO₃ is given as;

Figure 4.5 (a) Electron Density for BaSnO₃

The very first graph is for the BaSnO₃ in which symmetric is shown for the electrons density when magnetic field is absence, the main center portion shows combine effect of Ba-Sn, the light green color is for the oxygen representation, the upper corner shows Ba-O interactions and Sn-O shows lower corner interaction [21, 31, 32].

4.5.3 Band Gap

It can be defined as:

The energy of the states in which the electrons are found or exists are called Energy bands or Allowed Gap. On the other hand, those energy states in which the electrons cannot be exists are called Forbidden Gaps or Electronic Band Gaps [28].

The graph for the band structure for the BaSnO₃ is also studies by use of the Wien2k package are given as:

This graph is highly symmetric with the symmetric points of the Brillion Zone. With presence of the Electric field[31, 32], the different color and the curves shows the path of Electrons in Motions. Each curve shows the independent path of the electrons. The value of the energy is plotted against y-axis and, those of negative value

Figure 4.6 Band Gap for BaSnO₃

shows the energy below the fermi level which are valence and lower bands [21, 22, 33].

Those bands above the fermi levels are positive values showing conduction bands.

The graph is shown for the BaSnO₃ which seems to same band structure throughout the structure thus showing BaSnO₃ is a unique compound. In the graph the symmetry points are plotted along x-axis. In BaSnO₃ the maximum points of the valence band are shown in grey color lies in M symmetry point whereas the minimum points are lies in Γ symmetry points, are purple in color which seems BaSnO₃ is categories as indirect Band Gap Compound. It is also named as M- Γ Indirect Band Gap Compound [17, 34-38].

Wide bandgap perovskite oxides with high room temperature conductivities and structural compatibility with a diverse family of organic/inorganic perovskite materials are of significant interest as transparent conductors and as active components in power electronics. Such materials must also possess high room temperature mobility to minimize power consumption and to enable high-frequency applications.

Acknowledgements:

Corresponding Author: Zubair Ashraf (+923082528918)
Email: Zubair@stu.pku.edu.cn

The authors are thankful to the Lab facilities provided by University of the Punjab. There is no conflict of interest between authors.

5.0 References:

1. Blaha, P., et al., *WIEN2k: An APW+lo program for calculating the properties of solids*. J Chem Phys, 2020. **152**(7): p. 074101.
2. Athawale, A.A., M.S. Bapat, and P.A. Desai, *Hydrothermal preparation of BaSnO₃ and Au-BaSnO₃ nanorods*. J Nanosci Nanotechnol, 2008. **8**(8): p. 4258-62.
3. Prakash, A., et al., *Wide bandgap BaSnO₃ films with room temperature conductivity exceeding 10(4) S cm(-1)*. Nat Commun, 2017. **8**: p. 15167.
4. Arezoomandan, S., et al., *THz characterization and demonstration of visible-transparent/terahertz-functional electromagnetic structures in ultra-conductive La-doped BaSnO₃ Films*. Sci Rep, 2018. **8**(1): p. 3577.

Corresponding Author: Zubair Ashraf (+923082528918)
Email: Zubair@stu.pku.edu.cn

5. Buannic, L., et al., *Probing cation and vacancy ordering in the dry and hydrated yttrium-substituted BaSnO₃ perovskite by NMR spectroscopy and first principles calculations: implications for proton mobility*. J Am Chem Soc, 2012. **134**(35): p. 14483-98.
6. Donval, G., et al., *A hybrid method using the widely-used WIEN2k and VASP codes to calculate the complete set of XAS/EELS edges in a hundred-atoms system*. Phys Chem Chem Phys, 2017. **19**(2): p. 1320-1327.
7. Eustace, D.A., D.W. McComb, and A.J. Craven, *Probing magnetic order in EELS of chromite spinels using both multiple scattering (FEFF8.2) and DFT (WIEN2k)*. Micron, 2010. **41**(6): p. 547-53.
8. Hebert, C., *Practical aspects of running the WIEN2k code for electron spectroscopy*. Micron, 2007. **38**(1): p. 12-28.
9. Galazka, Z., et al., *Melt growth and properties of bulk BaSnO₃ single crystals*. J Phys Condens Matter, 2017. **29**(7): p. 075701.
10. Hebert, C., J. Luitz, and P. Schattschneider, *Improvement of energy loss near edge structure calculation using Wien2k*. Micron, 2003. **34**(3-5): p. 219-25.
11. Holec, D., et al., *Electron energy loss near edge structure (ELNES) spectra of AlN and AlGaIn: a theoretical study using the Wien2k and Telnes programs*. Micron, 2008. **39**(6): p. 690-7.
12. Huang, C., et al., *A facile peroxo-precursor synthesis method and structure evolution of large specific surface area mesoporous BaSnO₃*. Inorg Chem, 2015. **54**(8): p. 4002-10.
13. Kim, D.W., et al., *BaSnO₃ perovskite nanoparticles for high efficiency dye-sensitized solar cells*. ChemSusChem, 2013. **6**(3): p. 449-54.
14. Kim, M., et al., *Oxygen-Vacancy-Introduced BaSnO₃-delta Photoanodes with Tunable Band Structures for Efficient Solar-Driven Water Splitting*. Adv Mater, 2019. **31**(33): p. e1903316.
15. Kim, Y.M., et al., *Interface polarization model for a 2-dimensional electron gas at the BaSnO₃/LaInO₃ interface*. Sci Rep, 2019. **9**(1): p. 16202.
16. Lee, J.H., et al., *Transparent p-CuI/n-BaSnO₃-delta heterojunctions with a high rectification ratio*. J Phys Condens Matter, 2017. **29**(38): p. 384004.
17. Zhu, L., et al., *Mesoporous BaSnO₃ layer based perovskite solar cells*. Chem Commun (Camb), 2016. **52**(5): p. 970-3.
18. Allam, O., et al., *Density Functional Theory - Machine Learning Approach to Analyze the Bandgap of Elemental Halide Perovskites and Ruddlesden-Popper Phases*. Chemphyschem, 2018. **19**(19): p. 2559-2565.

19. Azam, S., et al., *Revealing the optoelectronic properties of Re-based double perovskites using the Tran-Blaha modified Becke-Johnson with density functional theory*. J Mol Model, 2020. **26**(6): p. 158.
20. English, N.J., *Dynamical properties of organo lead-halide perovskites and their interfaces to titania: insights from Density Functional Theory*. Heliyon, 2020. **6**(3): p. e03427.
21. Xiao, Z., et al., *Correction to "Intrinsic Instability of Cs₂In(I)M(III)X₆ (M = Bi, Sb; X = Halogen) Double Perovskites: A Combined Density Functional Theory and Experimental Study"*. J Am Chem Soc, 2017. **139**(27): p. 9409.
22. Xiao, Z., et al., *Intrinsic Instability of Cs₂In(I)M(III)X₆ (M = Bi, Sb; X = Halogen) Double Perovskites: A Combined Density Functional Theory and Experimental Study*. J Am Chem Soc, 2017. **139**(17): p. 6054-6057.
23. Mizoguchi, H., et al., *Strong near-infrared luminescence in BaSnO₃*. J Am Chem Soc, 2004. **126**(31): p. 9796-800.
24. Nahm, H.H., et al., *Amorphous Mixture of Two Indium-Free BaSnO₃ and ZnSnO₃ for Thin-Film Transistors with Balanced Performance and Stability*. ACS Appl Mater Interfaces, 2020. **12**(3): p. 3719-3726.
25. Ovcharov, A.V., et al., *Microstructure and superconducting properties of high-rate PLD-derived GdBa₂Cu₃O_{7-δ} coated conductors with BaSnO₃ and BaZrO₃ pinning centers*. Sci Rep, 2019. **9**(1): p. 15235.
26. Prakash, A., et al., *Separating Electrons and Donors in BaSnO₃ via Band Engineering*. Nano Lett, 2019. **19**(12): p. 8920-8927.
27. Rajamanickam, N., et al., *Efficiency enhancement of cubic perovskite BaSnO₃ nanostructures based dye sensitized solar cells*. Phys Chem Chem Phys, 2016. **18**(12): p. 8468-78.
28. Sanchela, A.V., et al., *Thermopower Modulation Clarification of the Operating Mechanism in Wide Bandgap BaSnO₃-SrSnO₃ Solid-Solution Based Thin Film Transistors*. Small, 2019. **15**(8): p. e1805394.
29. Shin, S.S., et al., *Colloidally prepared La-doped BaSnO₃ electrodes for efficient, photostable perovskite solar cells*. Science, 2017. **356**(6334): p. 167-171.
30. Wang, W.Y., et al., *Atomic mapping of Ruddlesden-Popper faults in transparent conducting BaSnO₃-based thin films*. Sci Rep, 2015. **5**: p. 16097.
31. Wang, Y., et al., *High-mobility two-dimensional electron gas in SrGeO₃- and BaSnO₃-based perovskite oxide heterostructures: an ab initio study*. Phys Chem Chem Phys, 2016. **18**(46): p. 31924-31929.

32. Wu, M., et al., *The Role of Annealing Process in Ag-Based BaSnO₃ Multilayer Thin Films*. Nanoscale Res Lett, 2016. **11**(1): p. 369.
33. Yue, J., et al., *Depletion Mode MOSFET Using La-Doped BaSnO₃ as a Channel Material*. ACS Appl Mater Interfaces, 2018. **10**(25): p. 21061-21065.
34. Yun, H., et al., *Microstructure characterization of BaSnO₃ thin films on LaAlO₃ and PrScO₃ substrates from transmission electron microscopy*. Sci Rep, 2018. **8**(1): p. 10245.
35. Yun, H., et al., *STEM beam channeling in BaSnO₃/LaAlO₃ perovskite bilayers and visualization of 2D misfit dislocation network*. Ultramicroscopy, 2020. **208**: p. 112863.
36. Yun, H., et al., *Metallic line defect in wide-bandgap transparent perovskite BaSnO₃*. Sci Adv, 2021. **7**(3).
37. Zhang, Y., M.P. Sahoo, and J. Wang, *Tuning the band gap and polarization of BaSnO₃/SrSnO₃ superlattices for photovoltaic applications*. Phys Chem Chem Phys, 2017. **19**(10): p. 7032-7039.
38. Zhang, Y., et al., *Strain-induced ferroelectricity and lattice coupling in BaSnO₃ and SrSnO₃*. Phys Chem Chem Phys, 2017. **19**(38): p. 26047-26055.

Figures

Figure 1

The basic cubic structure of Perovskites.

Figure 2

An Ore of Barium

Figure 3

An ore of Tin

Figure 4

Oxygen in liquid form

Figure 5

Introduction to Wien2k

Figure 6

ideal cubic unit cell of BaSnO3

Figure 7

The total energies of the cell volume of BaSnO3

Figure 8

(a) Electron Density for BaSnO3

Figure 9

Band Gap for BaSnO3

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- [GraphicalAbstractnew1.docx](#)