COMPUTATIONAL STUDY OF ANTIMONY SULPHIDE ABSORBANCE LAYER FOR SOLAR CELLS

AFIQ BIN RADZWAN

UNIVERSITI TEKNOLOGI MALAYSIA

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AFIQ BIN RADZWAN

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ABSTRACT

The demand for cheaper, nontoxic and earth-abundant materials as absorbing layer for solar cell is immensely needed to replace scarce, toxic and expensive one. In this regard, chalcogenide materials have attracted the attention of a lot of researchers because of their great potential in different applications. Antimony sulphide (Sb_2S_3), a chalcogenide binary material is investigated to exploit its potential for different energy technologies being a less toxic, abundantly available, stable and efficient, which are the fundamentals for sustainability as well as to realize the dream of green energy. Theoretical calculations based on density functional theory (DFT) are employed to study and understand the structural, electronic and optical properties of Sb_2S_3 for three-dimensional (3-D), two-dimensional (2-D) and one-dimensional (1-D) structures. Here, the investigations have been performed by full-potential linearized augmented plane-wave method (FP-LAPW) within the WIEN2k computational code. The optical properties such as imaginary and real parts of the dielectric function, absorption coefficient, refractive index, reflectivity, and electron energy loss function are analyzed. In 3-D structure study, lattice parameters obtained are comparable to the experimental measurements. The obtained indirect energy band gap of 1.63 eV and optical properties are also closer to the experimental data. As the dimensions and size changed, the physical properties of Sb_2S_3 are also changed. The indirect energy band gaps obtained for 2-D and 1-D structures of Sb_2S_3 are 0.57 eV and 0.12 eV, respectively which are smaller than 3-D Sb_2S_3. The investigation of thickness effect on 2-D Sb_2S_3 is presented. The obtained values of indirect energy band gaps for various levels were found to be 0.568, 0.596 and 0.609 eV for 1, 2 and 4 levels, respectively. The density of state (DOS) illustrated for both 2-D and 1-D structures are higher than 3-D structure. The obtained absorption coefficients for both Sb_2S_3 structures are around 10^4 cm^{-1} in the visible light and ultraviolet regions. The static refractive index calculated for 3-D, 2-D and 1-D structures are 3.05, 1.77 and 1.48, respectively. From these results, it is clearly shown that 2-D and 1-D Sb_2S_3 structures have lower optical properties than 3-D Sb_2S_3. However, the absorption coefficients of 2-D and 1-D Sb_2S_3 structures are considerably higher and reflect their potentiality for photovoltaic applications.

ABSTRAK

Tuntutan bahan yang murah, tidak bertoksik dan paling banyak di Bumi sebagai lapisan penyerap di dalam sel suria adalah sangat diperlukan bagi menggantikan bahan yang susah didapati, toksik dan mahal. Berkenaan perkara ini, bahan kalkogenida telah menarik perhatian ramai penyelidik kerana potensi yang besar untuk pelbagai aplikasi tenaga. Antimoni sulfida (Sb_2S_3), bahan kalkogenida biner telah dikaji untuk mengeksploitasi potensinya untuk teknologi tenaga berbeza yang kurang toksik, senang didapati, tersedia, stabil dan cekap, yang merupakan asas kepada kelestarian dan juga untuk merealisasikan impian tenaga hijau. Pengiraan teori berdasarkan teori fungsian ketumpatan (DFT) telah digunakan untuk mengkaji dan memahami sifat-sifat struktur, elektronik dan optik Sb_2S_3 untuk struktur tiga-dimensi (3-D), dua-dimensi (2-D) dan satu-dimensi (1-D). Di sini, penyiasatan dilakukan menggunakan kaedah keupayaan penuh gelombang satah terimbuh (FP-LAPW) dalam kod perkomputeran WIEN2K. Sifat-sifat optik seperti bahagian khayal dan nyata fungsi dielektrik, pekali penyerapan, indeks biasan, keterpantulan dan fungsi kehilangan tenaga elektron telah dianalisa. Dalam kajian struktur 3-D, dapatan parameter kekisi adalah setanding dengan pengukuran eksperimen. Dapatan jurang jalur tenaga tidak langsung 1.63 eV dan sifat optik juga hampir dengan data eksperimen. Dengan perubahan dimensi dan saiz, sifat fizikal Sb_2S_3 juga berubah. Dapatan jurang jalur tenaga tidak langsung untuk 2-D dan 1-D Sb_2S_3 masing-masing ialah 0.57 eV dan 0.12 eV yang mana ia adalah lebih kecil berbanding 3-D Sb_2S_3. Penyiasatan kesan ketebalan ke atas 2-D Sb_2S_3 telah dibentangkan. Dapatan jurang jalur tenaga tidak langsung untuk beberapa tahap didapati 0.568, 0.596 dan 0.609 eV untuk tahap 1, 2 dan 4. Ketumpatan keadaan (DOS) yang ditunjukkan untuk kedua-dua struktur 2-D dan 1-D Sb_2S_3 adalah lebih kecil berbanding struktur 3-D. Dapatan pekali penyerapan untuk kedua-dua struktur 2-D dan 1-D Sb_2S_3 ialah dalam linkungan $10^4 cm^{-1}$ dalam rantau cahaya nampak dan ultraungu. Indeks biasan statik struktur 3-D, 2-D dan 1-D Sb_2S_3 yang dikira masing-masing ialah 3.05, 1.77 dan 1.48. Daripada hasil kajian, ia jelas menunjukkan struktur 2-D dan 1-D Sb_2S_3 mempunyai sifat-sifat optik yang lebih rendah berbanding 3-D Sb_2S_3. Walau bagaimanapun, pekali penyerapan struktur 2-D dan 1-D Sb_2S_3 adalah lebih tinggi dan mencerminkan potensi mereka dalam aplikasi fotovolta.

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LIST OF ABBREVIATIONS

1-D	-	One-Dimension
2-D	-	Two-Dimensional
3-D	-	Three-Dimensional
AlN	-	Aluminium Nitride
a-Si	-	Amorphous Silicon
BeO	-	Beryllium Oxide
Bi_2S_3	-	Bismuthinite
Bi_2Se_3	-	Guanajuatite
BZ	-	Brillouin Zone
CdTe	-	Cadmium Telluride
CIGS	-	Copper Indium Gallium Diselenide
CO_2	-	Carbon Dioxide
c-Si	-	Crystalline Silicon
DOS	-	Density of State
DSCs	-	Dye-Sensitized Cells
ETA	-	Extremely Thin Absorber
EV-GGA	-	Engel Vosko Generalized Gradient Approximation
FP	-	Full Potential
FP-LAPW	-	Full Potential Augmented Plane Wave
FTO	-	Fluorine-doped Tin Oxide
GaP	-	Gallium Phosphide
GaS	-	Gallium Sulfide
GaSe	-	Gallium Selenide
GWA	-	GW Approximation
HF	-	Hartree-Fock
HK	-	Hohenberg–Kohn
LDA	-	Local Density Approximation
MT	-	Muffin Tin
PBE-GGA	-	Perdew–Burke–Ernzerhof Parameterized Generalized Gradient Approximation

PBEsol-GGA	-	Perdew-Burke Ernzerhof Parameterized Generalized Gradient Approximation for Solids and Surfaces
PCE	-	Power Conversion Efficiency
PV	-	Photovoltaic
RPA	-	Random phase approximation
Sb_2S_3	-	Antimony Sulphide
Sb_2Se_3	-	Antimonselite
SCF	-	Self-Consistent Field
SOC	-	Spin Orbit Coupling
TB-mBJ	-	Tran-Blaha-Modified-Becke-Johnson
WC-GGA	-	Wu-Cohen Parameterized Generalized Gradient Approximation
ZnO	-	Zinc Oxide

LIST OF SYMBOLS

h	-	Planck's constant
μm	-	Micrometer
eV	-	Electron volt
cm^{-1}	-	Centimeter per ssecond
α	-	Absorption coefficient
nm	-	Nanometer
PPM	-	Parts per million
%	-	Percentage
Ψ	-	Schrödinger wavefunction
Φ	-	Electronic wavefunction
H	-	Hamiltonian
N	-	Number of atoms
m_i	-	Nuclei mass
m_e	-	Electron mass
$\vec{R}_i$	-	Nuclei position
$\vec{r}_i$	-	Electron position
e	-	Electron charge
Z	-	Atomic number
$\hat{T}$	-	Kinetic energy of electron
$\hat{T}_n$	-	Kinetic energy of nuclei
$\hat{V}_{ee}$	-	Coulomb interaction of electron-electron
$\hat{V}_{ext}$	-	Coulomb interaction of electron-nucleus
$\hat{V}_{nn}$	-	Coulomb interaction of nucleus-nucleus
E	--	Total energy
E_{elec}	-	Nuclear energy
E_{nuc}	-	Electronic energy
E_H	-	Hartree energy
ρ	-	Electron density
ρ_0	-	Electron ground-state density,

E_0	-	Ground-state energy
E_{KS}	-	Kohn-sham energy
ε_{XC}	-	Exchange correlation energy density
V_{XC}	-	Exchange correlation potential
V_{eff}	-	Effective potential
V_H	-	Hartree potential
$\widehat{H}_{KS}$	-	Kohn-sham hamiltonian
C_k^i	-	Coefficient of basis set
E_{XC}^{RPA}	-	Random phase approximation (RPA) exchange-correlation energy
ε_1	-	Real part of dielectric function
ε_2	-	Imaginary part of dielectric function
k	-	Reciprocal vector in brillouin zone
G	-	Reciprocal lattice vector
V_{cell}	-	Volume of unit cell
ρ_{in}	-	Initial electron density
ρ_{out}	-	Output electron density
$V_{x,\sigma}^{BJ}$	-	Becke-Johnson (BJ) exchange potential
$V_{x,\sigma}^{BR}$	-	Becke-Roussel (BR) exchange potential
$V_{x,\sigma}^{mBJ}$	-	Modified Becke-Johnson exchange potential
$\widehat{H}_{SO}$	-	Spin -orbit coupling hamiltonian
V_0	-	Equilibrium volume
B_0	-	Bulk modulus
B_1	-	First derivative of the bulk modulus with respect to pressure
P	-	Principal value of the integral in irreducible brillouin zone
ω	-	Frequency
n	-	Refractive index
R	-	Reflectivity
L	-	Loss function

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CHAPTER 1

INTRODUCTION

1.1 Background study

In the modern civilization, most of the global energy is produced from fossil fuels [1] mainly petroleum, natural gas and coal as described in Figure 1.1.

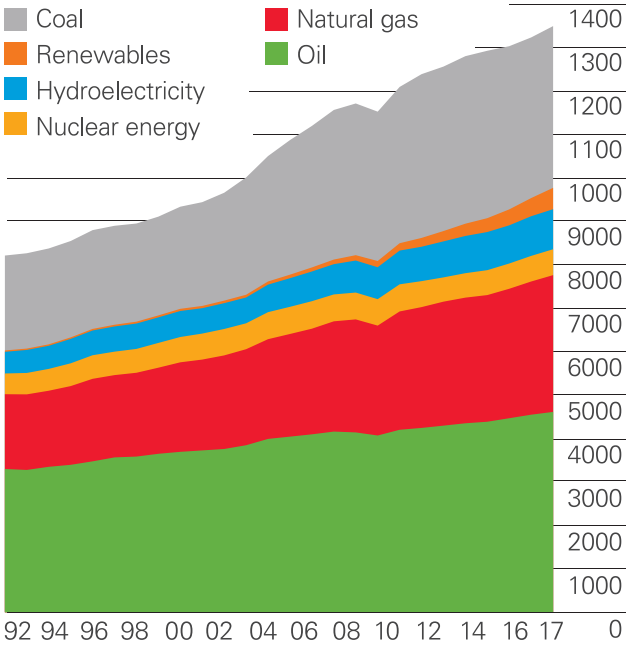

Figure 1.1 Primary global energy consumption according to the British Petroleum Company (BP) statistical review of global energy 2017 [1]

Unfortunately, the civilization's overuse leading to the rapid depletion of global energy resource supplies. The global energy consumption is expected to be increased at the rate of 1.5% [2]. Global consumption of fossil fuels increased 24% for coal, 20% for natural gas and 7.5% for petroleum from 2005 to 2014 [3]. Fossil fuels are also harmful for the environment. Emissions of carbon dioxide (CO_2) from the fossil fuel power plants are not only affecting the climate [4], but they also destroy wild habitats [5] and cause pollution problems [6], as well as serious human health

problems [7]. In 2017, global CO_2 emission from fossil fuels has risen by 1.6% and it is expected to go up by more than 2% in 2018 [8,9]. Considering energy is very important to modern society, therefore it is very important to find alternative energy resource such as renewable energy to satisfy the world sustainable and clean energy demand [10]. In 2017, global investors around the world invested 279.8 billion USD in the development of renewable energy technologies [11].

Among renewable resources, solar energy has great potential for sustainable and clean energy production due to its abundance and free of CO_2 emission [12]. Installation of 113,533 household solar cells in California, USA, have reduced 696,544 metric tons of CO_2 emissions [13]. According to M. Hosenuzzaman, et al. [14], the use of solar cells can lower 69–100 million tons of CO_2 by 2030. The Sun emits solar energy at a rate of about 3.8×10^{26} kW [12]. This energy can be harvested with solar cell [15]. Solar cells are devices that convert photon energy of sunlight into useful electricity. Schematic system of photovoltaic (PV) solar energy is shown in Figure 1.2.

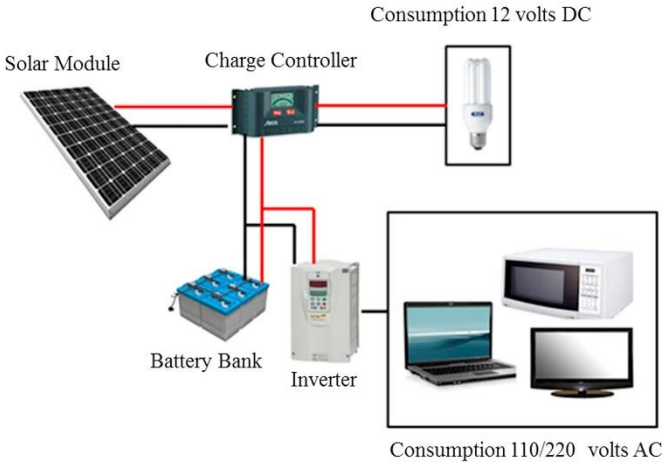

Figure 1.2 Typical system of photovoltaic (PV) solar energy [16].

Solar cells based on semiconductor have shown great performance due to its unique physical properties. The first generation of solar cells were developed based on semiconductor crystalline silicon (c-Si) [17] and gallium arsenide (GaAs) [18]. The first generation of solar cells are wafer-based solar cell. However, GaAs are too expensive for terrestrial large-area applications because of the availability of rare of gallium (Ga) element. The average estimated crustal abundance of gallium is generally

less than 19 parts per million (ppm) [19]. Currently c-Si based solar cells have dominated solar cell market because of their performance. In 2017, crystalline silicon solar cells have dominated around 95% of the solar market [20]. As well understood silicon is, non-toxic, earth-abundant and stable. Note that natural abundance of Si is 25.7 ppm which much higher than Ga [21]. However, due its complex process of purifying for solar-grade silicon from its raw source made the production expensive [22]. The cost of pure crystalline silicon is about 40-60% of the solar cell manufacturing cost. Average manufacturing cost of a silicon-based solar cell is $0.38 per watt and selling price of $0.44 per watt in 2015 [23]. To install solar power at large scales, huge plots of land are often required. About 16,187 m^2 of land area would require for a 1MW solar power plant [24].

In the search for cost reduction for solar cells, second-generation solar cell has been developed as absorber layer in solar cells. Currently, Amorphous silicon (a-Si) [25], cadmium Telluride (CdTe) [26], and copper indium gallium diselenide (CIGS) [27] are the leading materials in second generation solar cells. These materials have higher absorption than crystalline silicon (c-Si) [28,29] and close to the ideal material for photovoltaic conversion. These types of solar cells are considered as the second generation of solar cell. However, until now, c-Si solar cell has the highest power conversion efficiency (PCE) [30]. As shown in Figure 1.3, the higher efficiency solar cells are GaAs and c-Si. The efficiency of CdTe and CIGS are 21.0 % and 21.7 % respectively [30]. The major factor that contributing to this issue is the band gap of the semiconductor material. c-Si has a nearly ideal band gap (1.34 eV) [31] to absorb the maximum photons from the sun's radiation [32]. Currently, second generation solar cell may suffer from issues of availability [33] and toxicity [34] ,if widely used. The estimated crustal abundance of cadmium (Cd), indium (In), tellurium (Te) and selenium (Se) are 0.098 ppm, 0.05 ppm, 0.001 ppm and 0.05 ppm respectively [35]. Hence, the price of these materials has increased because of their low abundance in the earth’s crust. The price of Cd, In, Te and Se are 100 $/kg, 700 $/kg, 168 $/kg and 300 $/kg respectively [35]. The In materials are the most expensive due to its application in liquid crystal display (LCD) screen technology. The toxicity of thin film solar cells came from cadmium (Cd). Cadmium poisoning is one of the global health problems that affect many organs and it can cause deaths. Long-term exposure to cadmium can leads to organ system toxicity and cancer [36].Hence, Cadmium based

technologies should be restricted to a minimal or no harmful level. Thus, alternative materials for solar cell which are cheaper, abundant, and less toxic need to be developed.

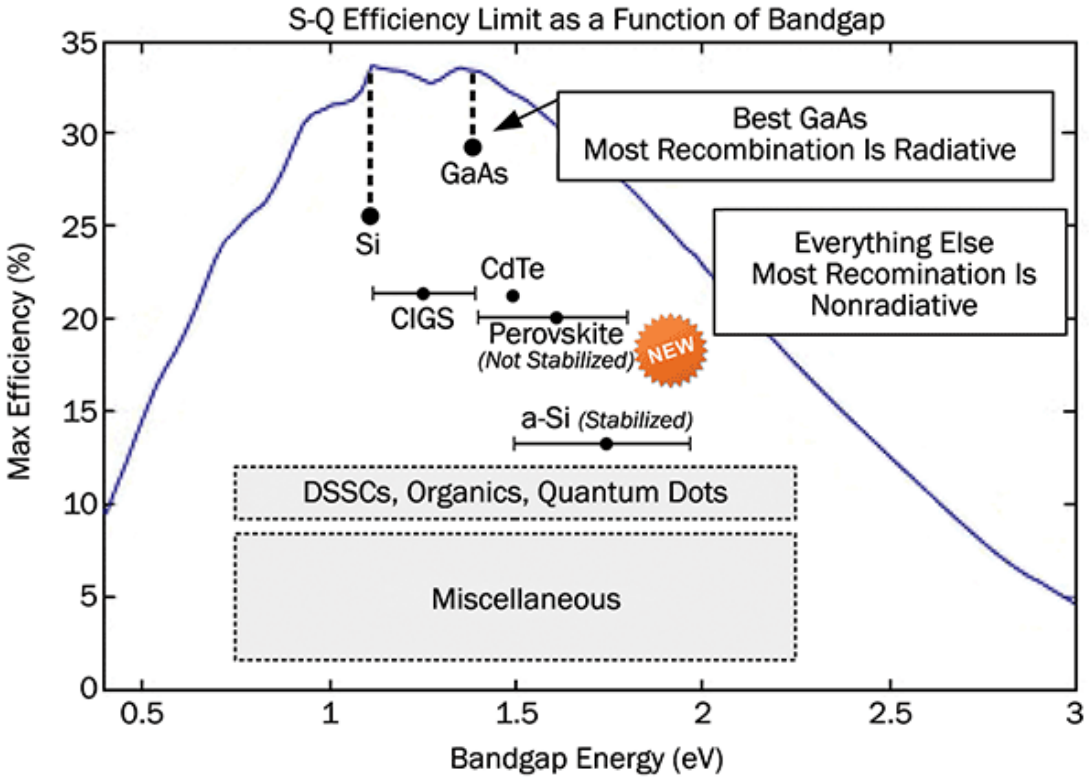

Figure 1.3 Theoretical Shockley-Queisser (S-Q) detailed-balance efficiency limit as a function of band gap [37].

Third generation of solar cell [38] was developed to overcome the issues in first- and second-generation solar cells. Third-generation solar cells usually refer to technologies that promise to be even cheaper than previous generations. Third-generation solar cells include organic materials, dye-sensitized solar cells (DSSCs) and perovskite solar cell. However, third-generation solar cells are still in development and not been widely marketed. The efficiency of third generation solar cells are between 9.7% to 20.9% [30]. DSSCs are formed by porous layer of titanium dioxide (TiO_2) nanoparticles (inorganic), covered with a molecular dye (organic) that absorbs photon [39]. The highest efficiency has been reported so far is only 11.9% [30]. However, organic molecular dye used suffers instability problems. Instead of using a molecular dye, extremely thin absorber (ETA) layer of a small band gap semiconductor can be used as absorber [40]. The efficiency of 4.9% has been achieved [41]. However,

semiconductor sensitized solar cells (SSSC) are much less reported than the DSSC but are attracting increasing interest. Some researchers consider other semiconductor as the alternative to TiO_2 such as (1 dimensional) 1-D zinc oxide (ZnO) [42] and 1-D Si [43]. The efficiency of 1-D ZnO and 1-D Si are 7.13% and 0.253%. However, these efficiencies are not high enough for commercial application.

Sham L.J. [44] and Xiao H. [45] have shown that the computational method density functional theory (DFT) is a suitable method in calculating the electronic structure of semiconductor materials. DFT has been used to study material for solar cell application such c-Si [46], CdTe [47] and CIGS [48]. Recent years, DFT has been used to study low-dimensional structure [49–51].

1.2 Problem statements

Several material candidates from chalcogenide group compound materials such as CdTe and CIGS are promising materials for photovoltaic applications, because of their appropriate energy gaps and photoconductive properties [52]. Among the metal chalcogenides group which a semiconductor material, antimony sulphide (Sb_2S_3) has gained intensive research for optoelectronic devices in various form. Sb_2S_3 satisfied the requirement future generation of solar cells. Due to strong optical properties, Sb_2S_3 is suitable 2-D solar cell [53–61]. However, their PCE is not high as other commercial solar cells [62]. Several studies found that Sb_2S_3 extremely thin absorber has shown the most encouraging results to replace photoactive dyes in dye-sensitized solar cells [53,63–65]. The highest solar cell efficiency obtained for DSSCs is 7.5% [30]. However, the band gaps obtained are varied due to the fabrication methods used. From the literatures, Sb_2S_3 have good electrical properties [66–73]. Sb_2S_3 are among several candidates to be considered as replacement of TiO_2 in DSSC [74]. Many physical properties exhibit strong dependence on their size and dimensionality [75,76]. However, this effect is rarely reported due to limited study on Sb_2S_3 and some optical properties also are not revealed. Thus, optical properties of Sb_2S_3 are not well understood. 1-D Sb_2S_3 shows a small band gap closer to ideal band gap for solar cell material compared to its other forms. The potential of Sb_2S_3 as

absorber in for photovoltaic (PV) solar cell is unclear due to the challenge and limitation in experimental study.

There are areas in material studies that are not accessible by experiment such as the electronic structure. In spite of the various applications proposed for Sb_2S_3, very little is known of its electronic structure. It is well recognized that the electronic structure of solids plays a very effective tool in determining their properties [77]. Density functional theory (DFT) has been well used for investigating electronic structure in semiconductor [44,45]. There are numerous computational studies of 3-D Sb_2S_3 using DFT that have been done [78,79,88,80–87] but there are only several studies reported on the optical behaviour of this compound. Hence, relationship between electronic structure and optical properties are not well understood. Moreover, the computational study on low dimensional Sb_2S_3 such as 2-D and 1-D structures are highly rare so far due to its complex and disordered structure. There are only two theoretical studies on low dimensional Sb_2S_3 [79,86]. However, Chen, J.H. et al. did not calculate the optical properties and Caruso, F. et al. did not present the density of state (DOS) which both are essential for optoelectronic application study. Thus, the effects of dimensionality reduction on electronic structure are unclear. Some experimental studies [89,90] observed the changes in physical properties of 2-D Sb_2S_3 with changes in thickness. However, the thickness dependence in Sb_2S_3 has not been discussed theoretically. Hence, the study of electronic structure for different structure of Sb_2S_3 is critical. There are numerous exchange correlation approximations have been proposed to enhance the accuracy of DFT calculation [91,92]. However, only a few exchange correlation approximations have been used in DFT calculations of Sb_2S_3. The performance of exchange correlation approximation on optical properties of Sb_2S_3 also unclear.

The spin-orbit coupling (SOC) in DFT calculation is usually ignored due to the small effect but, it is substantial. For heavy element such as antimony (Sb). However, there is not very much study regarding to this matter. Currently, only two DFT studies on Sb_2S_3 has been done with inclusion of SOC [82,86]. However, that is only in 3-D level. The SOC effect is different for each dimensional structure [93]. The effect of SOC in low dimensional Sb_2S_3 structure is unknown.

1.3 Research Objectives

To resolve the above-mentioned issues, this study embarks on the following objectives:

(a) To calculate the electronic and optical properties of Sb_2S_3 using different approximations.

(b) To determine the effect of thickness in electronic and optical properties of Sb_2S_3.

(c) To determine the effect of spin orbit coupling (SOC) in electronic band gap of Sb_2S_3.

(d) To identify the potential of Sb_2S_3 as absorber in photovoltaic (PV) solar cell.

1.4 Research Scope

The investigation of the structural, electronic and optical properties in three-dimensional (3-D), two-dimensional (2-D) and one-dimensional (1-D) of Sb_2S_3 structures will be performed using a computational method based on DFT [94–96]. The 3-D, 2-D and 1-D structures are included in this study. The WIEN2k code [97–101] based on full potential augmented plane wave (FP-LAPW) methodology will be used to analyse structural, electronic, and optical properties of each structure. The spin orbit coupling is included for 3-D, 2-D and 1-D structures calculations.

Investigation of the structural optimization of 3-D Sb_2S_3 is carried out by employing local density approximation (LDA), Engel Vosko generalized gradient approximation (EV-GGA), Perdew‑Burke‑Ernzerhof parameterized generalized gradient approximation (PBE-GGA), Wu-Cohen parameterized GGA (WC-GGA) and Perdew-Burke Ernzerhof parameterized generalized gradient approximation for solids and surfaces (PBEsol-GGA) exchange correlation functional. But the investigation of the electronic and optical properties of 3-D Sb_2S_3 are carried out by employing above-

mentioned exchange-correlation functionals with addition of Tran-Blaha-modified-Becke-Johnson (TB-mBJ).

Computational study on 2-D and 1-D Sb_2S_3 structures are carried out using optimized unit cell from 3-D calculation. The investigation electronic and optical of 2-D Sb_2S_3 with thickness of 1 level (1.16 nm) is carried out using LDA, PBE-GGA, EV-GGA. However, thickness effect study on 2-D Sb_2S_3 is carried out using EV-GGA only. The thickness is increased from 1 to 8 levels. For 1-D Sb_2S_3, the investigation of electronic and optical of with diameter of several nanometers is carried out using EV-GGA.

1.5 Significance of Study

The successful execution of this FP-LAPW method can open avenues for designing the novel materials, and moreover, can provide a guideline to the industrial sector for synthesizing cost-effective novel materials for energy efficient technologies and save energy thus provide a safe environment. Furthermore, DFT provide the properties that cannot reach by experimental method. Additionally, this study reveals much clear optical properties of Sb_2S_3 explain the relationship between electronic structure and optical behaviour. Besides, the intention of this study is to present the accurate procedure of first principles to calculate the electronic structure in low-dimensional structure level. However, due to the limit of computation, the physical properties of Sb_2S_3 in various form cannot be explored widely. Furthermore, the properties studied in this project is limited. However, results obtained are enough to give proper understanding the effect of dimensionality and size reduction. These efforts hoped can stimulate more research on solar cell materials.

1.6 Thesis Organization

This thesis is categorized into five different chapters. Chapter 1 describes the importance of harvesting solar energy and solar cell technology. Furthermore, the

problem statements, research objectives, scope of research, significance of study and thesis organization are defined in this chapter. Chapter 2, the overview of the literature related to the research title. This chapter covers fundamental of solar cell, the experimental and theoretical studies on Sb_2S_3 and lastly DFT method. Next, the Chapter 3 provides the details of WIEN2K package and procedure of calculation.as well as the detail of calculation for 2-D and 1-D Sb_2S_3 structures. Chapter 4 discusses the structural, electronic and optical properties of 3-D Sb_2S_3. The effect of SOC is also included in this chapter as well as the detailed discussion for electronic and optical of 2-D and 1-D Sb_2S_3 structures. The effect of thickness on 2-D Sb_2S_3 is also discussed in the end of this chapter. Finally, in the Chapter 5, the general conclusion along with recommendation are discussed. At the end of thesis, the list of reference and appendix are presented.

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LIST OF PUBLICATIONS

1. **Radzwan, A**., Ahmed, R., Shaari, A., Lawal, A. and Ng, Y.X., (2017). First-principles calculations of antimony sulphide Sb2S3. *Malaysian Journal of Fundamental and Applied Sciences*, *13*(3), 285-289. https://doi.org/10.11113/mjfas.v13n3.598
2. **Radzwan, A**., Ahmed, R., Shaari, A., Ng, Y. X., & Lawal, A. (2018). First-principles calculations of the stibnite at the level of modified Becke–Johnson exchange potential. *Chinese Journal of Physics*, *56*(3), 1331-1344. https://doi.org/10.1016/j.cjph.2018.03.005 **(Q3, IF: 1.051)**
3. **Radzwan, A**., Ahmed, R., Shaari, A. and Lawal, A., (2019). Ab initio calculation of antimony sulphide nanowire. *Physica B: Condensed Matter*. *557*, 17-22. https://doi.org/10.1016/j.physb.2019.01.005 **(Q3, IF: 1.453)**
4 **Radzwan, A**., Ahmed, R., Shaari, A. and Lawal, A., (2019). Ab initio calculations of optoelectronic properties of antimony sulfide nano-thin film for solar cell applications. *Results in Physics*, *15*, 102762. https://doi.org/10.1016/j.rinp.2019.102762
5 **Radzwan, A**., Ahmed, R., Shaari, A. and Lawal, A., (2020). First-principles study of electronic and optical properties of antimony sulphide thin film. *Optik*, *202*, 163631. https://doi.org/10.1016/j.ijleo.2019.163631