

## Device Simulation of $\text{Sb}_2\text{S}_3$ Solar Cells by SCAPS-1D Software

ODARI, Victor <sup>1,2a\*</sup>, MUSEMBI, Robinson <sup>1, b</sup> and MWABORA Julius <sup>1, c</sup>

<sup>1</sup>Department of Physics, School of Physical Sciences, University of Nairobi, P.O. Box 30197-00100 Nairobi, Kenya.

<sup>2</sup>Department of Physics, School of Natural and Applied Sciences, Masinde Muliro University of Science and Technology, P.O. Box 190-50100 Kakamega, Kenya.

<sup>a</sup>vodari@mmust.ac.ke\*, <sup>b</sup>musembirj@uonbi.ac.ke, <sup>c</sup>mwabora@uonbi.ac.ke

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### ABSTRACT

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Antimony sulphide ( $\text{Sb}_2\text{S}_3$ ) has drawn research interest due to its promising properties for photovoltaic applications. The progress in developing highly efficient  $\text{Sb}_2\text{S}_3$  solar cells has stimulated this study to a great extent. In this paper, we present the results of a simulation of solar cell processing parameters on the performance of the solar cell through theoretical analysis and device simulation using SCAPS software. The results of this simulation show that the solar cell performance can be enhanced to a great extent by adjusting the thickness, doping concentration and defect density of both the  $\text{TiO}_2$  buffer layer and  $\text{Sb}_2\text{S}_3$  absorber layer and also the electron affinity of the  $\text{TiO}_2$  buffer layer. Optimized parameters were found to be: doping concentration of ( $1.0 \times 10^{17} \text{cm}^{-3}$  for  $\text{TiO}_2$  and  $3.0 \times 10^{16} \text{cm}^{-3}$  for  $\text{Sb}_2\text{S}_3$ ), defect density of the  $\text{Sb}_2\text{S}_3$  absorber at ( $1.0 \times 10^{15} \text{cm}^{-3}$ ) and the electron affinity of the buffer layer at (4.26 eV). The results obtained were as follows:  $V_{oc}$  of 750 mV,  $J_{sc}$  of  $15.23 \text{ mA/cm}^2$ , FF of 73.55% and efficiency of 8.41%. These results show that  $\text{Sb}_2\text{S}_3$  is a potential earth-abundant compound that can yield highly efficient solar cells.

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## 1. Introduction

Antimony sulphide ( $\text{Sb}_2\text{S}_3$ ) is a chalcogenide semiconductor with promising properties for photovoltaic applications such as its suitable band gap, relatively non-toxic and earth-abundant constituent, simple composition (binary compound), and long term stability [1].

It is a V–VI semiconductor material and exists in nature in the form of the mineral stibnite with orthorhombic crystal structure (lattice parameters  $a = 1.1239$ ;  $b = 1.1313$ ; and  $c = 0.38411$  nm) [2]. It has been widely used in electronic applications such as thermoelectric devices, photo-electrochemical cells, microwave devices, switching devices and photodetectors [3]. Various techniques such as thermal evaporation [3–6], chemical bath deposition [7–10], spin coating [11], spray pyrolysis, sputtering [12] and electrodeposition [13] have been used to deposit  $\text{Sb}_2\text{S}_3$  thin films. Depending on the method of synthesis, both p-type and n-type conductivity have been reported for  $\text{Sb}_2\text{S}_3$  thin films [13].

Many research groups have demonstrated the use of  $\text{Sb}_2\text{S}_3$  as an absorber material either as a planar or a sensitized solar cell [3, 12]. Efficiencies up to 1.27% have been reported using thermally evaporated  $\text{Sb}_2\text{S}_3$  absorber layer [2]. [11] report an approach based thermal decomposition of  $\text{Sb(III)(thioacetamide)}_2\text{Cl}_3$  that yielded solar cells with a short-circuit current density of  $8.12 \text{ mAcm}^{-2}$  and an efficiency of 2.39% [11]. [14] reported a conversion efficiency of 5.1% for aqueous  $\text{Sb}_2\text{S}_3$  deposited at room temperature by CBD. [14] and [15] reported  $\text{Sb}_2\text{S}_3$  by CBD on nanoporous  $\text{TiO}_2$  and organic hole transporting material yielded an efficiency of 5.2%. [8] reported a photocurrent density of  $16.3 \text{ mA/cm}^2$  and power conversion efficiency of 5.7% for a glass/FTO/ $\text{TiO}_2$ / $\text{Sb}_2\text{S}_3$ /CuSCN/Au structure using  $\text{Sb}_2\text{S}_3$  doped with 5 at% Ti as a thin absorber film [8]. The highest efficiency of 7.5% has been achieved with a  $\text{TiO}_2$ / $\text{Sb}_2\text{S}_3$  based heterojunction system of the type: mesoporous- $\text{TiO}_2$ / $\text{Sb}_2\text{S}_3$ /PCPDTBT (poly(2,6-(4,4-bis-(2-ethylhexyl)-4Hcyclopenta[2,1b;3,4-b'] dithiophene)-alt-4,7(2,1,3-benzothiadiazole)))/Au [16].

In spite of the improvement in efficiencies of the  $\text{Sb}_2\text{S}_3$  based solar cells, to date, there has been no report on their device simulation which can apprise experimentalist on the possible maximum limit for this material. Simulation methods allow instinctive analysis of each parameter in solar cells and thus identify the optimal conditions of operation [17 - 18]. This study therefore focuses on factors that affect the performance of planar  $\text{Sb}_2\text{S}_3$  based solar cells which include film thickness, defect density and doping density variation of  $\text{Sb}_2\text{S}_3$  absorber layer and the thickness, doping density and electron affinity of the  $\text{TiO}_2$  buffer layer using the one-dimensional device simulation with the solar cell capacitance simulator (SCAPS) version 3.3.03 [19] under AM1.5G illumination. SCAPS is based on three semiconductor equations and can model various homo-junctions, hetero-junctions, multi-junctions and Schottky barrier devices [17].

## 2. Numerical Modeling and Material Parameters

The one dimensional SCAPS software [19] allows simulation of planar devices. The  $\text{Sb}_2\text{S}_3$  based planar solar cell with layer configuration of glass substrate/TCO/Buffer layer of  $\text{TiO}_2$  /absorption layer  $\text{Sb}_2\text{S}_3$ /hole transport material (HTM) P3HT/ Ag back contact is shown in figure 1. The material parameters of the different layers have been selected from those reported in theoretical and experimental data of other works [20]. Table 1 summarizes the parameters of each layer in the architecture and also indicates the parameters that were optimized for better results.  $\text{Sb}_2\text{S}_3$  is said to have a number of defects which include sulphur vacancies and antimony interstitials [21]. Therefore, we set the absorption characteristic energy at 0.1 eV and introduce two levels antisite defects  $\text{Sb}_{\text{S}_2}$  in the band gap, one donor at  $\epsilon_{\text{SbS } 2 (+/0)} = 0.28 \text{ eV}$  and one acceptor at  $\epsilon_{\text{SbS } 2 (0/-)} = 0.53 \text{ eV}$ , which are both above VBM and should dislocate  $E_F$  near the VBM inducing p-type conductivity [21]. The initial defect density  $N_t$  of  $\text{Sb}_2\text{S}_3$  absorber material is set to  $5.000\text{E}+14$  [16]. The defects in  $\text{Sb}_2\text{S}_3$  as outlined by [21] show a p-type conducting behavior.

*Device Simulation of Sb<sub>2</sub>S<sub>3</sub> Solar Cells by SCAPS-1D Software*

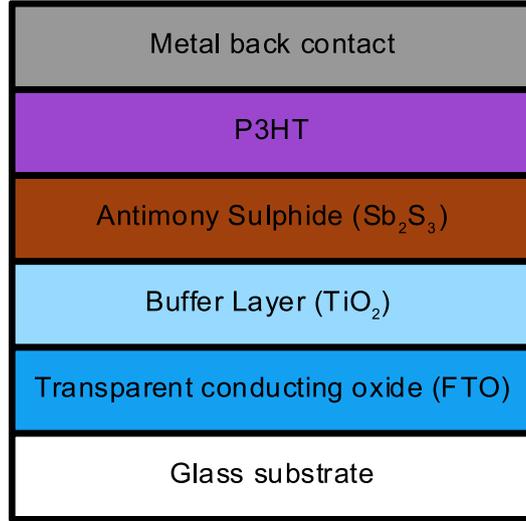


Figure 1: Cell architecture of planar Sb<sub>2</sub>S<sub>3</sub> based solar cell

Table 1. Layer parameters for the different layers of a Sb<sub>2</sub>S<sub>3</sub>-based solar cell at 300 K.

Parameter	Units	FTO	cp-TiO <sub>2</sub>	Sb <sub>2</sub> S <sub>3</sub>	P3HT
<b>E<sub>g</sub> (Band gap)</b>	eV	3.5	3.2	1.7	2
<b>χ<sub>e</sub> (Electron affinity)</b>	eV	4.4	4.26 (Varied)	3.8	3.2
<b>w (Thickness)</b>	nm	500	50 (Varied)	80 (Varied)	100
<b>ε<sub>r</sub> (Permittivity)</b>		9	11.9	7	3
<b>μ<sub>n</sub> (electron mobility)</b>	cm <sup>2</sup> /Vs	20	20	7.0×10 <sup>-2</sup>	6.0×10 <sup>-2</sup>
<b>μ<sub>p</sub> (hole mobility)</b>	cm <sup>2</sup> /Vs	10	10	2.0×10 <sup>-2</sup>	1.0×10 <sup>-2</sup>
<b>N<sub>c</sub> (Effective density of states in the conduction band)</b>	cm <sup>-3</sup>	2.2×10 <sup>18</sup>	2.2×10 <sup>18</sup>	1.0×10 <sup>19</sup>	1.0×10 <sup>19</sup>
<b>N<sub>v</sub> (Effective density of states in the valence band)</b>	cm <sup>-3</sup>	1.8×10 <sup>19</sup>	1.8×10 <sup>19</sup>	1.0×10 <sup>19</sup>	1.0×10 <sup>19</sup>
<b>N<sub>A</sub> (Carrier density of the acceptor)</b>	cm <sup>-3</sup>	0	0	3.0×10 <sup>16</sup> (Varied)	3.0×10 <sup>16</sup>
<b>N<sub>D</sub> (Carrier density of the donor)</b>	cm <sup>-3</sup>	2.0×10 <sup>19</sup>	1.0×10 <sup>16</sup>	0	0

We, therefore, assume that the absorber is p-type semiconductor with initial carrier density of 3.000E+16 cm<sup>-3</sup>. We have also introduced bulk defects in each layer as shown in Table 2. The interface defect at the TiO<sub>2</sub>/Sb<sub>2</sub>S<sub>3</sub> interface is set to be a neutral defect with a total density of 2.50E+17 [22] and single energetic distribution below the lowest E<sub>c</sub> as shown in Table 3.

The absorption coefficient ( $\alpha$ ) curve is calculated from  $\alpha = A_{\alpha}(h\nu E_g)^{1/2}$  with the pre-factor  $A_{\alpha}$  set to  $10^5$ .

Table 2. Parameters for the Gaussian distributed defect states in the different layers of  $\text{Sb}_2\text{S}_3$  solar cell.

	Units	FTO	cp-TiO <sub>2</sub>	Sb <sub>2</sub> S <sub>3</sub>
<b>Type</b>		Neutral	Neutral	Donor
<b>Density of defects</b>	cm <sup>-3</sup>	1×10 <sup>+15</sup>	1×10 <sup>+15</sup>	Varied from 10 <sup>10</sup> to 10 <sup>19</sup>
<b>Electron capture cross-section (<math>\sigma_n</math>)</b>	cm <sup>2</sup>	1×10 <sup>-15</sup>	1×10 <sup>-19</sup>	1.34×10 <sup>-17</sup>
<b>Hole capture cross-section (<math>\sigma_p</math>)</b>	cm <sup>2</sup>	1×10 <sup>-15</sup>	1×10 <sup>-19</sup>	1.34×10 <sup>-17</sup>
<b>Energy</b>	eV	Above E <sub>v</sub>	Above E <sub>v</sub>	Above E <sub>v</sub>

Table 3. Interface properties in  $\text{Sb}_2\text{S}_3$  solar cells.

	Interface	TiO <sub>2</sub> /Sb <sub>2</sub> S <sub>3</sub>
<b>Parameter</b>	Type	Neutral
<b>Density of defects</b>	cm <sup>-2</sup>	2.50×10 <sup>17</sup>
<b>electron capture cross-section (<math>\sigma_n</math>)</b>	cm <sup>-2</sup>	2.21×10 <sup>-9</sup>
<b>hole capture cross section (<math>\sigma_p</math>)</b>	cm <sup>-2</sup>	2.21×10 <sup>-9</sup>
<b>Energy</b>	eV	Below the lowest E <sub>c</sub>

Table 4 shows the solar cell parameters of the best cell of  $\text{Sb}_2\text{S}_3$  [16] that has so far been reported and the parameters of our simulated cell that mimic it using the initial parameters in table 1. The short-circuit current density ( $J_{sc}$ ) of 14.77 mA/cm<sup>2</sup>, open-circuit voltage ( $V_{oc}$ ) of 711.1 mV, fill factor (FF) of 71.82% and power conversion efficiency (PCE) of 7.54% are obtained. These simulated device parameters differ by a negligible error with the experimental values indicating that the device simulation is valid and the input parameters that have been set are close to those for a real device.

Table 4. Simulation and experiment parameters of a  $\text{Sb}_2\text{S}_3$  cell.

	V <sub>oc</sub> (mV)	J <sub>sc</sub> (mA/cm <sup>2</sup> )	FF (%)	$\eta$ (%)
Experiment [16]	711	16.1	65	7.5
SCAPS Simulation	711.1	14.77	71.82	7.54

### 3. Results and Discussions

#### 3.1 Effect of buffer layer thickness on the $J$ - $V$ characteristics

The simulation started by setting the thickness of  $Sb_2S_3$  layer to 200 nm and varying the thickness of the  $TiO_2$  buffer layer from 40 nm to 200 nm. It was observed that an increase in the thickness of the buffer layer leads to deteriorating solar cell properties as seen in figure 1. The significant change in the  $V_{oc}$ ,  $FF$  and efficiency of the cells is as a result of increase in the length of the electron pathways in  $TiO_2$  which in extreme cases causes decrease in  $J_{sc}$ . This change in  $V_{oc}$  can also be due to unnecessary increase in the total  $TiO_2$  surface area, causing electron back transfer reaction as shown in Figure 2.  $J_{sc}$  can also decrease because fewer photons penetrating to the  $Sb_2S_3$  absorber layer when the thickness of the buffer layer is increased as shown in the graph of quantum efficiency in Figure 3. The generated charges need to have a longer lifetime to be extracted through the  $TiO_2$  buffer layer but that is not possible. Consequently, there is increase in charge recombination occurring slightly at the absorber layer and more in the buffer layers as shown in Figure 4 as a result of increase in diffusion length with increase in  $TiO_2$  thickness. Thin buffer layers of less than 40 nm may not be achieved experimentally due to instruments limitations or the required fabrication techniques [18, 23]. Therefore, the range of 40 nm to 50 nm is the preferred optimized thickness of the  $TiO_2$  buffer layer for  $Sb_2S_3$  based solar cell.

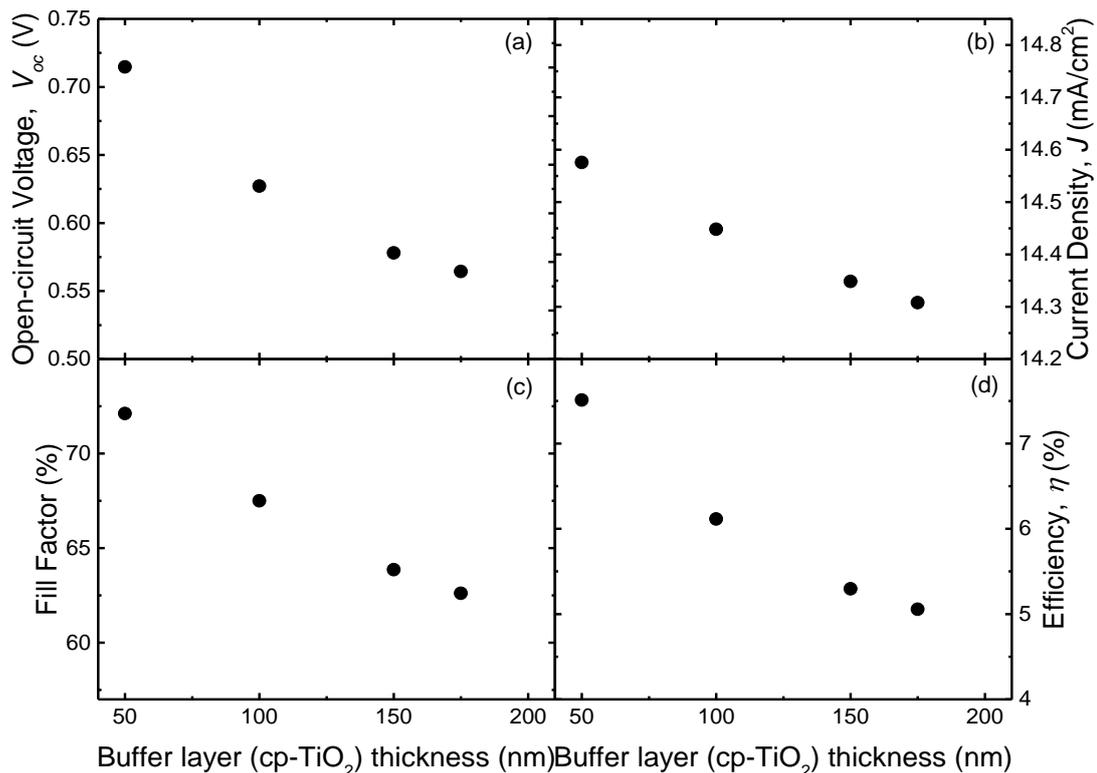


Figure 2: Variation in solar cell parameters with thickness of the buffer layer. There is increase in recombination at the  $TiO_2$  layer due to the short carrier lifetime with increase in thickness.

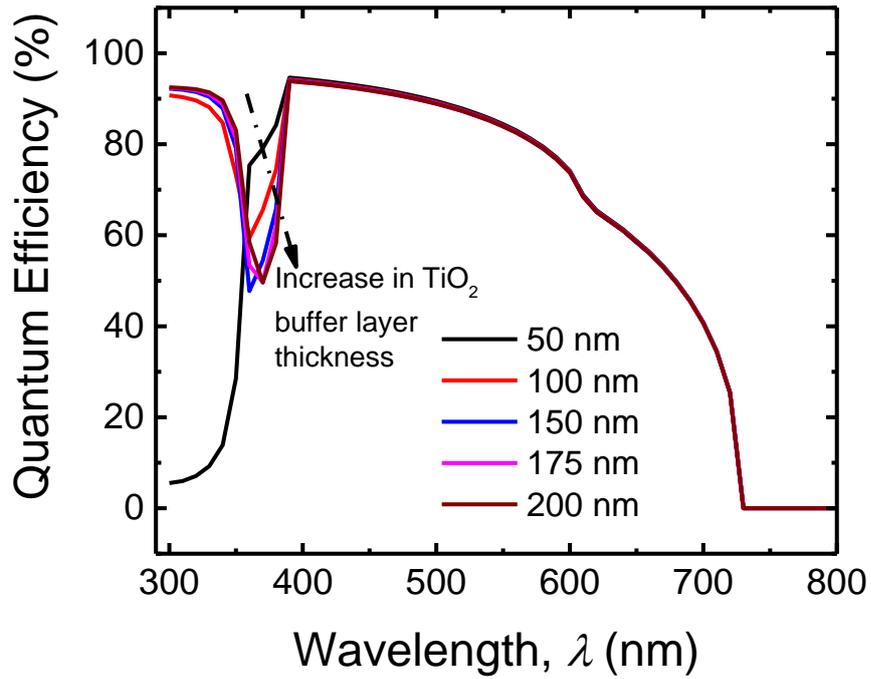


Figure 3: Quantum efficiency for  $Sb_2S_3$  solar cells with varying thickness of the  $TiO_2$  buffer layer

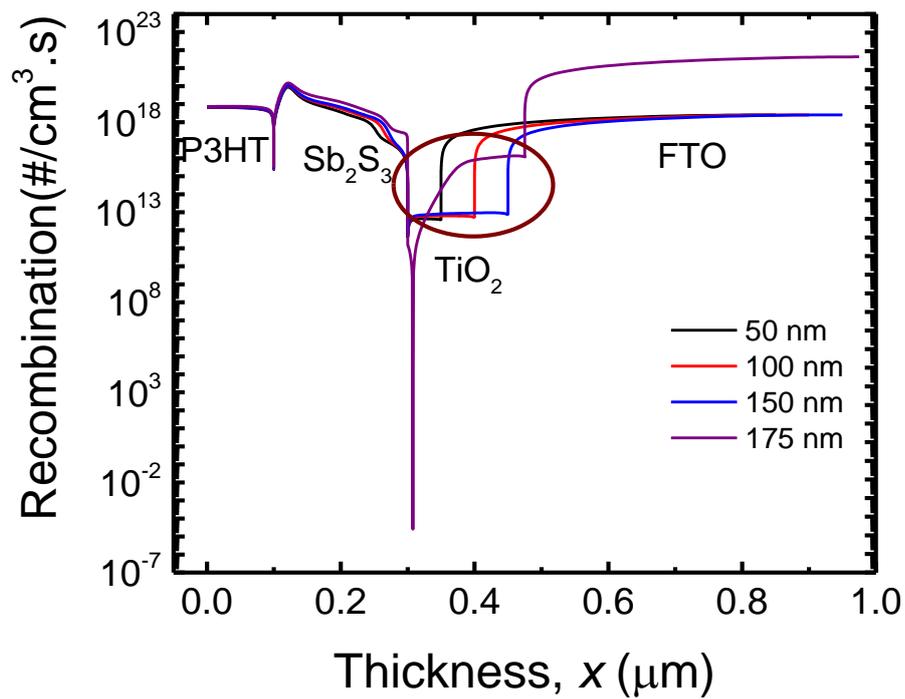


Figure 4: Recombination of charges with increase in buffer layer thickness

### 3.2 Effect of varying buffer layer ( $TiO_2$ ) doping density

Figure 5 shows increase in the doping density of the buffer layer results in improvement in the open-circuit voltage, fill factor and eventually the efficiency of the cells. Doping of the buffer layer mainly affects the reverse saturation current and the overall solar cell conversion efficiency.

**Device Simulation of  $Sb_2S_3$  Solar Cells by SCAPS-1D Software**

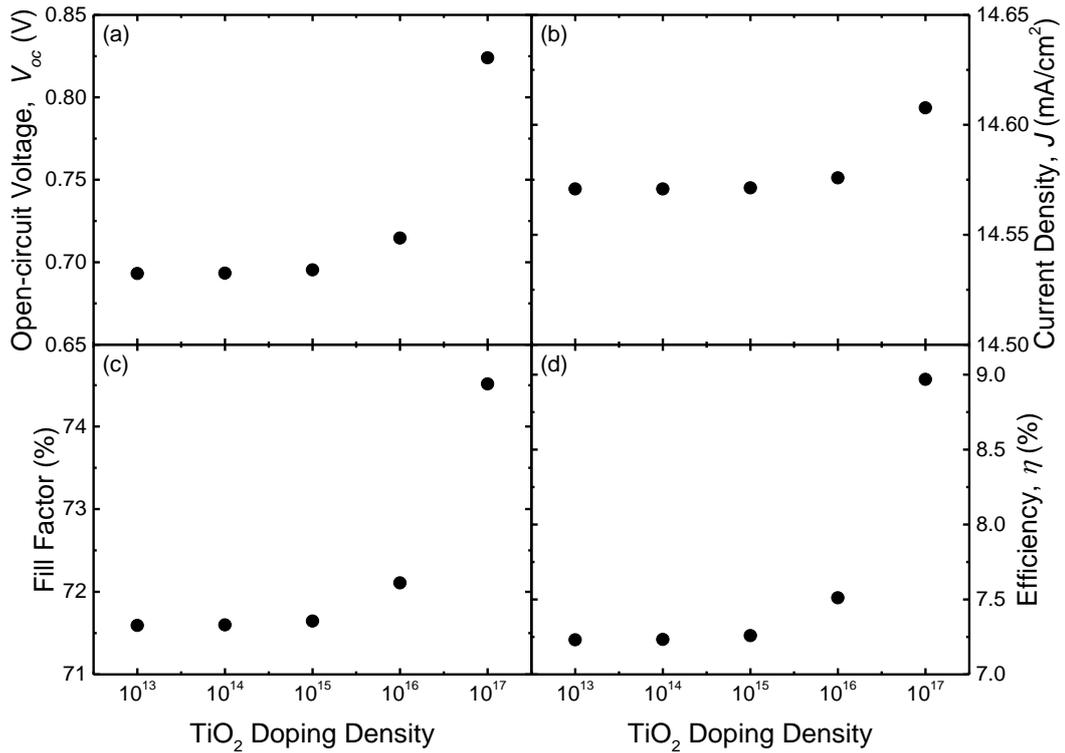


Figure 5: Variation in solar cell parameters with doping density of the buffer layer. Increase in the doping density leads to improved solar cell performance.

As the doping density increases from relatively small values of 10<sup>13</sup> per cm<sup>3</sup>, the reverse saturation current decreases leading to an increase in the open circuit voltage and consequently the conversion efficiency. This increase is sustained until the high doping effects appear causing a reduction of the band gap and the minority carrier life time which are expected to cause the reverse saturation current to decrease further after reaching a peak with the doping concentration in the TiO<sub>2</sub>. The slight decrease in band gap and minority carrier lifetime, therefore, leads to no significant change in the current density as shown by the graph of quantum efficiency in Figure 6. The doping concentrations as a process parameter therefore positively affects the open circuit voltage in the sense that the open circuit voltage increases by increasing the doping to an optimum value. These results show that doping densities of 10<sup>17</sup> per cm<sup>-3</sup> can yield solar cell efficiency of ~ 9% for the solar cell structure in Figure 1. Doping densities above this value may hardly change its carrier concentration given that TiO<sub>2</sub> is intrinsically an n-type semiconductor with high electron concentration.

It is expected that for an increase in defect density, both minority carrier lifetime and mobility should decrease causing a decrease in the open-circuit voltage but this has no effect on the TiO<sub>2</sub> buffer layer as shown in Figure 7.

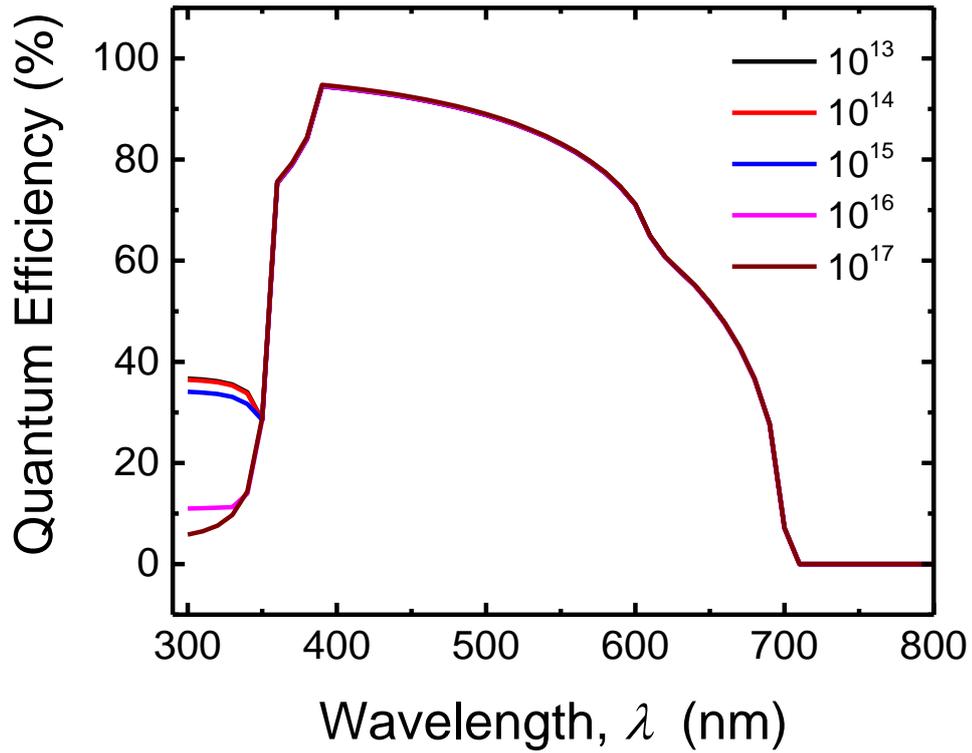


Figure 6: Quantum efficiency of solar cells with varying TiO<sub>2</sub> doping density.

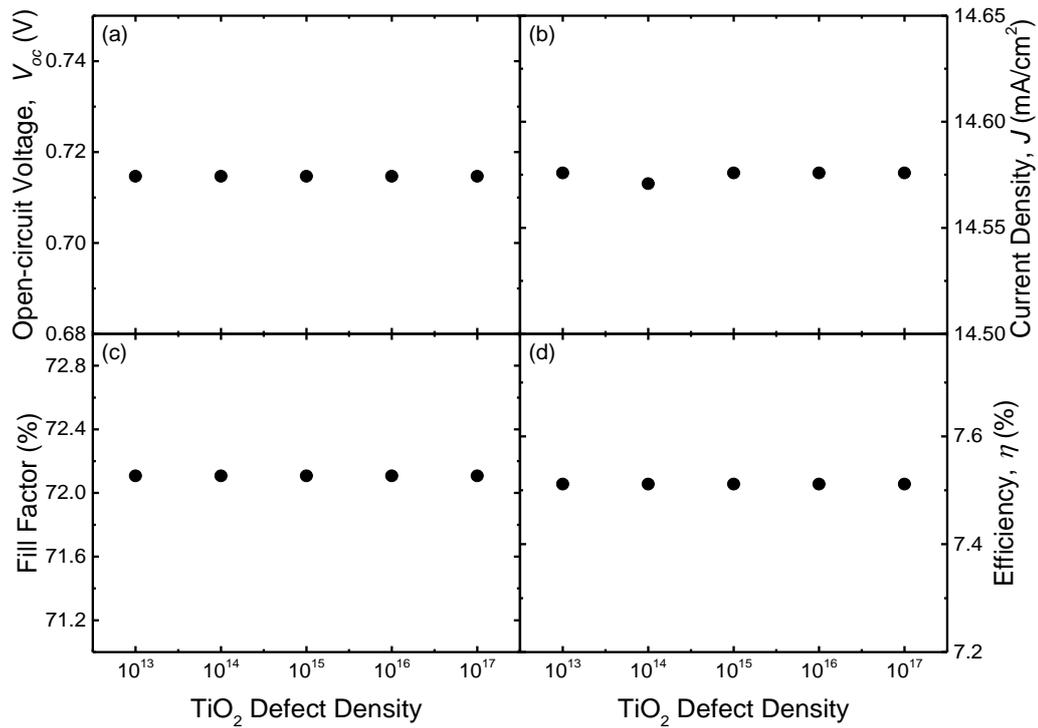


Figure 7: Graph on the effect of varying defect density of the TiO<sub>2</sub> buffer layer on the solar cell parameters.

### 3.3 Effect of varying buffer layer ( $TiO_2$ ) electron affinity

A critical factor of carrier recombination at the interface of semiconductors which determine the open-circuit voltage is the band offset between buffer/absorption layer/HTM [17]. We adjusted it by varying the values of electron affinity ( $\chi$ ) of the buffer from 3.5 eV to 4.7 eV. The variations of  $V_{oc}$ ,  $J_{sc}$ ,  $FF$ , and  $PCE$  with electron affinity value are shown in Figure 8. Satisfactory results of the solar cell parameters can be obtained at the  $\chi$  values of 3.5 eV– 4.2 eV for the buffer layer. A notch is formed on the hole Fermi level at the interface of the buffer layer and absorber as shown in the inset of Figure 9. The position of this notch with respect to the vacuum level, increases with increase in the electron affinity for energy values greater than 4.2 eV. The notch for the  $\chi$  values of 4.2 eV and 4.4 eV are -0.39eV and -0.28 eV respectively, indicating a high probability of carrier recombination at the interface hence causing a decrease in the  $V_{oc}$ .

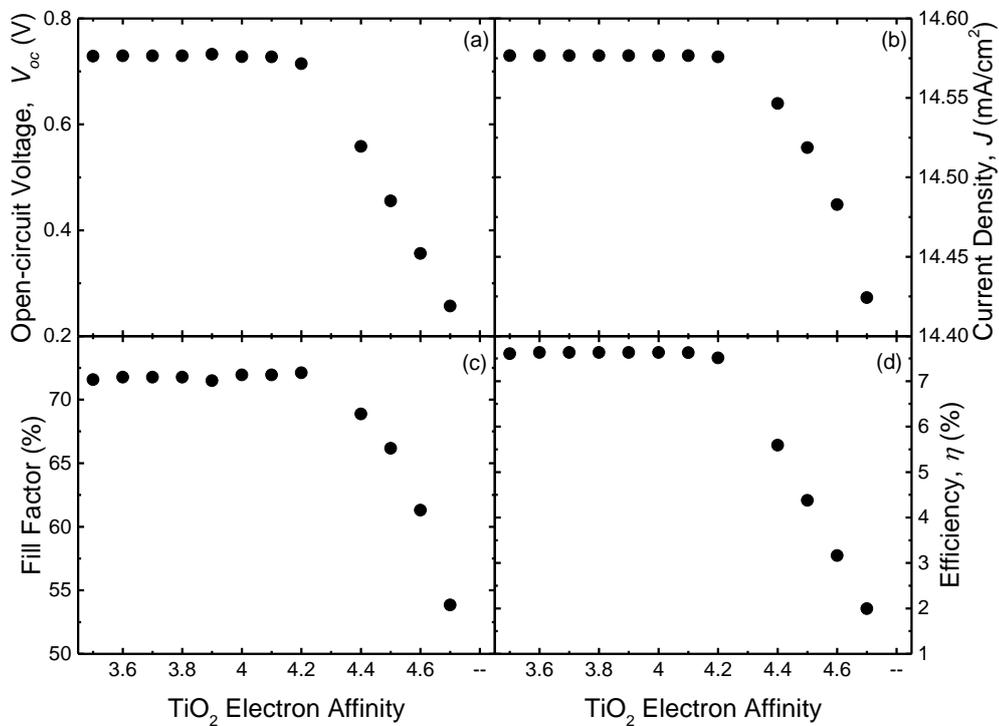


Figure 8: Variation in solar cell parameters with  $TiO_2$  electron affinity. There is no significant change in the cell parameters for layers with electron affinity of 4.2 eV and below.

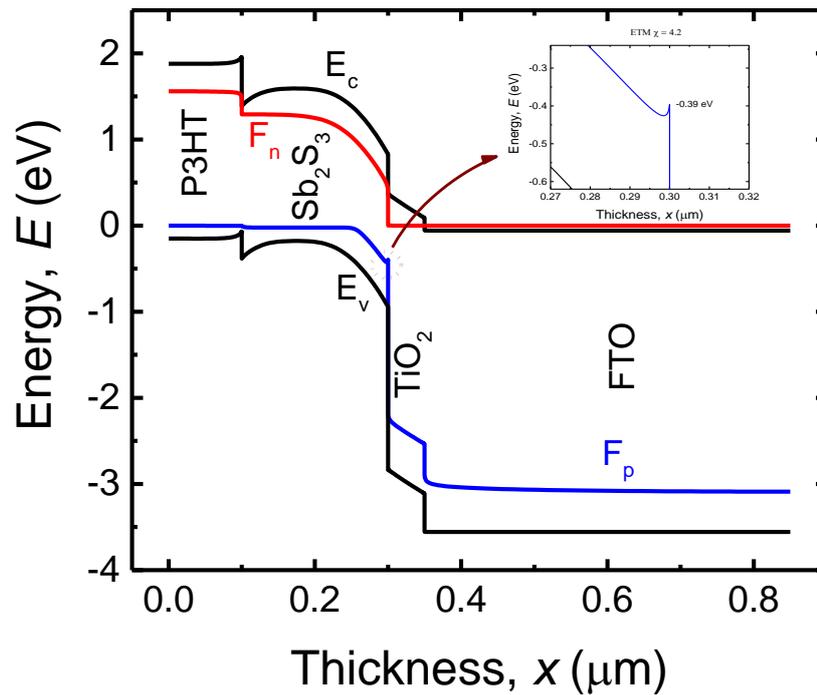


Figure 9: Band diagram of  $\text{Sb}_2\text{S}_3$  solar cell with  $\text{TiO}_2$  buffer layer

### 3.4 Effect of $\text{Sb}_2\text{S}_3$ thickness on the photovoltaic parameters

The thickness of the absorber layer plays an important role in charge extraction in thin films and the layer must be made sufficiently large to absorb all the penetrating incident radiation. This can be varied in the fabrication process. To obtain qualitative information, we have investigated the effects of  $\text{Sb}_2\text{S}_3$  layer thickness on the performance of the solar cells. Figure 10 shows variations in the solar cell parameters when varying the thickness of  $\text{Sb}_2\text{S}_3$  layer while keeping other layer properties constant. We observe that the  $V_{oc}$  and  $FF$  are nearly constant for thickness beyond 140 nm while the  $J_{sc}$  and the cell efficiency increase exponentially. Increase in thickness of the absorber layer, as expected, causes an increase in the short-circuit current resulting from more photons that are absorbed by  $\text{Sb}_2\text{S}_3$  layer. This also causes an increase in recombination of charges both at the interface of  $\text{Sb}_2\text{S}_3/\text{P3HT}$  and in the bulk of  $\text{Sb}_2\text{S}_3$  as seen in Figure 11. These recombination lead to a drop in the  $V_{oc}$  to a nearly constant value of 0.7 V for thickness beyond 140 nm. This value of thickness was also reported by [10] for chemically deposited n-type  $\text{Sb}_2\text{S}_3$  as the hole ambipolar diffusion length together with the electron diffusion length of  $\sim 1 \mu\text{m}$  [10]. The obtained almost constant  $V_{oc}$  is due to the recombination kinetics in  $\text{Sb}_2\text{S}_3$  is not expected to change when the diffusion length of charge carriers gets significantly lower than the thickness of the layer [10] implying that recombination is not affected by the surface states in  $\text{Sb}_2\text{S}_3$ . Recombination of the charge carriers is therefore due to defects at grain boundaries and in the bulk of the material.

Device Simulation of  $Sb_2S_3$  Solar Cells by SCAPS-1D Software

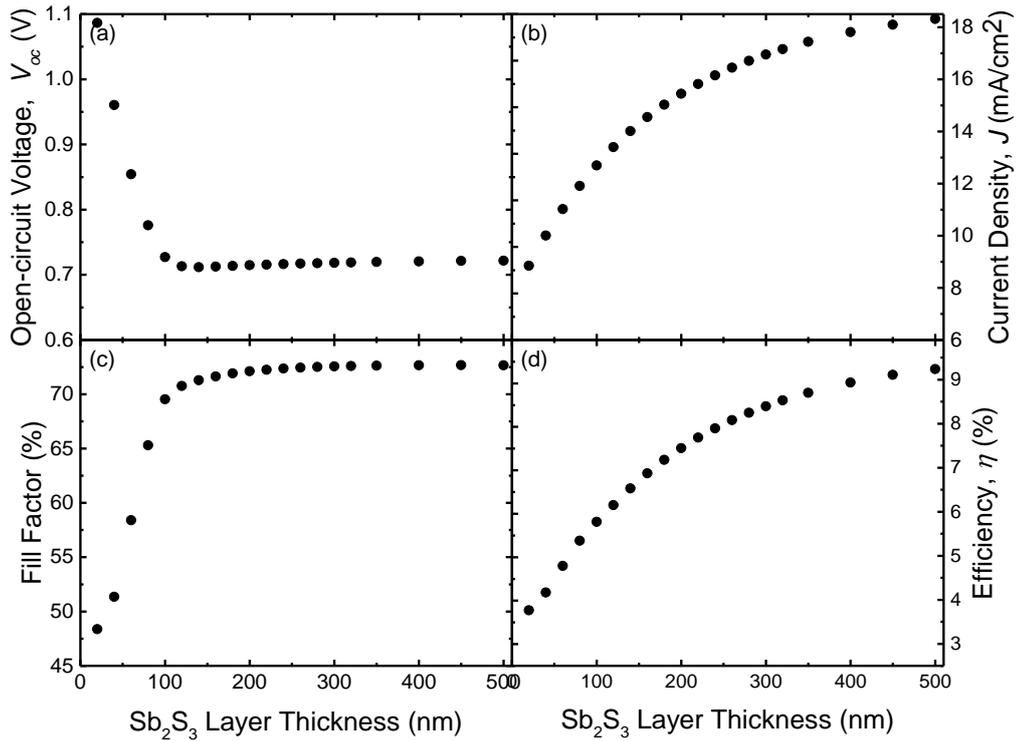


Figure 10: Variation in solar cell parameters with thickness of  $Sb_2S_3$ . Thicker films have a fairly constant output.

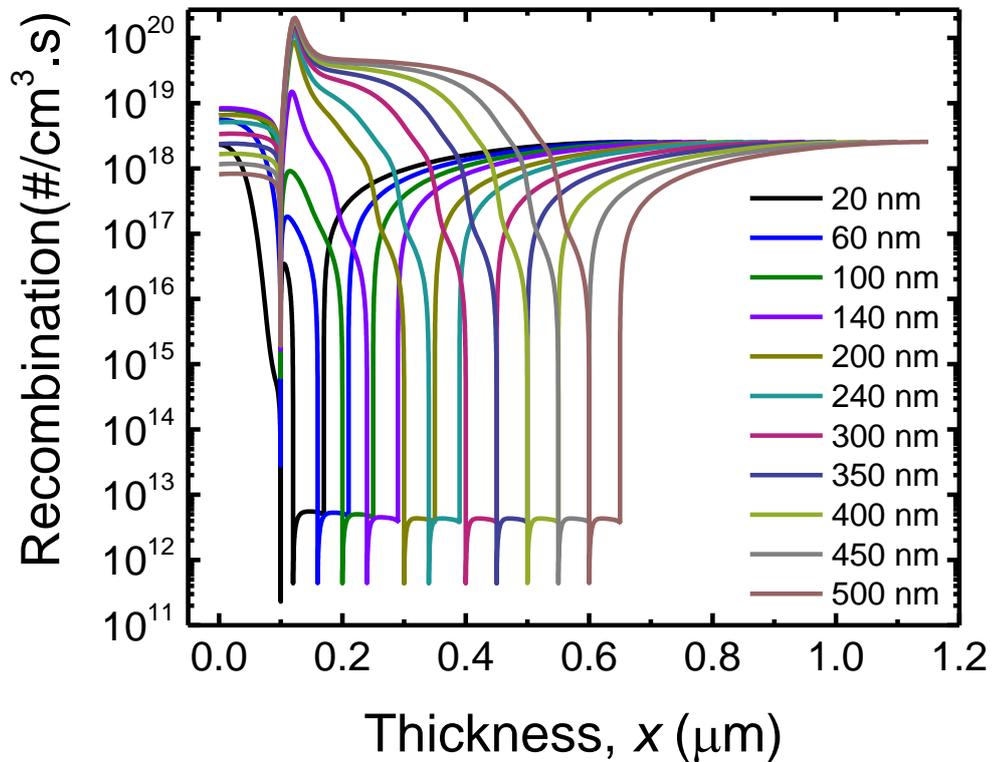


Figure 11: Recombination rate versus  $Sb_2S_3$  thickness.

### 3.5 Effect of $\text{Sb}_2\text{S}_3$ defects density on the photovoltaic parameters

Milton *et al.* [21] have theoretically studied the defect properties of  $\text{Sb}_2\text{S}_3$  using the density functional theory calculations in VASP software and reported on native point defects which may determine the type of  $\text{Sb}_2\text{S}_3$  semiconductor. Their study show that a p-type  $\text{Sb}_2\text{S}_3$  semiconductor can be obtained from low formation energy of antisite defects of  $\text{Sb}_5^2$  (Sb in place of S2 atom), introducing two levels in the band gap. These levels are a single donor (+/0) at 0.28 eV and a single acceptor (0/-) at 0.53 eV which are above the valence band maximum and will dislocate  $E_F$  near the VBM. Figure 12 presents the defect density effects on the solar cell performance parameters using the results obtained by Milton *et al.* The performance of the solar cell is at its best when the defects density is below  $10^{15} \text{ cm}^{-3}$ . When the defects density exceeds this value, the electrical performance of all the parameters are strongly affected. The presence of oxygen ions in chemical bath deposited  $\text{Sb}_2\text{S}_3$  may also introduce carrier traps which result in weak efficiency solar cells. Roy *et al.* [24] reported two activation energy for p-type  $\text{Sb}_2\text{S}_3$  of 0.40 and 0.22 eV which correlate to the donor level at 0.28 eV and acceptor level at 0.53 eV [16], [21] and are lower than its band gap (1.7 eV). Thus, close to deep defect levels, increase of defect density contributes to recombination loss mechanism. Therefore, fabrication of  $\text{Sb}_2\text{S}_3$  absorber materials with a high quality (defect density  $\sim 10^{15} \text{ cm}^{-3}$ ) is important for the  $\text{Sb}_2\text{S}_3$  based solar cell devices.

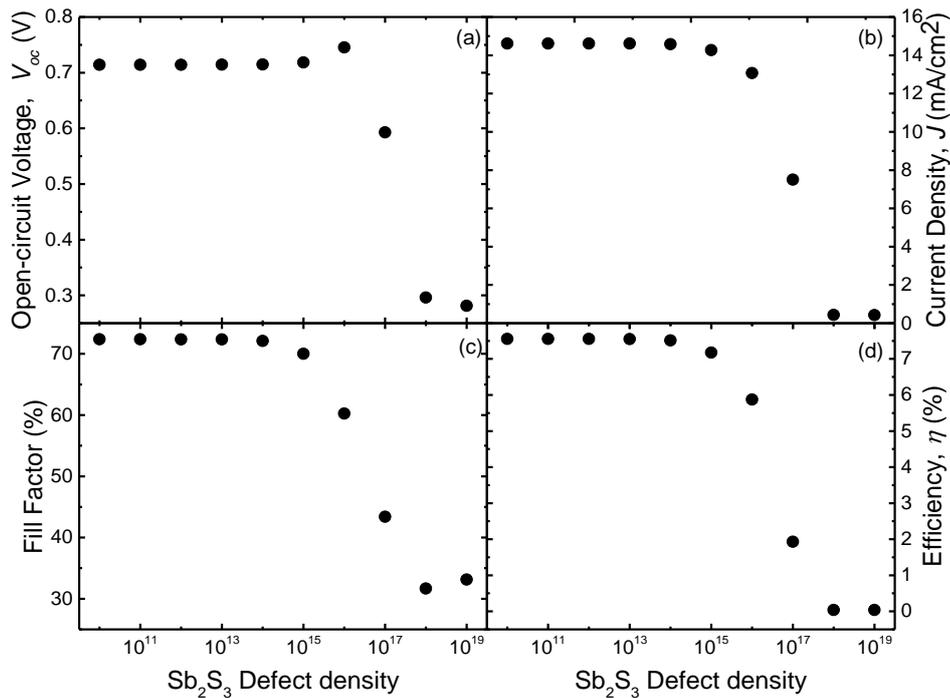


Figure 12: Variation in solar cell parameters with defect density of  $\text{Sb}_2\text{S}_3$ .

### 3.6 Effect of doping density in $\text{Sb}_2\text{S}_3$ solar cells

Figure 13 illustrates the influence of the holes' density ( $p$ ) on  $V_{oc}$ ,  $J_{sc}$ , FF, and efficiency of  $\text{Sb}_2\text{S}_3$  solar cell. We obtained a nearly constant open-circuit voltage of 0.9 V, short-circuit current of 13.9  $\text{mA/cm}^2$ , fill factor of 46% and efficiencies of 6% for doping densities of less than  $10^{14} \text{ cm}^{-3}$ . Doping densities higher than this value has improved solar cell parameters apart from the  $V_{oc}$ . Increase in doping densities reduces the trap density in  $\text{Sb}_2\text{S}_3$  and therefore improves on charge collection from the absorber.

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Doping densities above  $10^{14} \text{ cm}^{-3}$  will result in decrease in  $V_{oc}$  but with improvement in  $J_{sc}$ , FF and efficiency of the cells. This is a result of a shift in the Fermi levels towards the mid-gap hence lowering the  $V_{oc}$  and enabling easy excitation of charges. Doping densities above  $10^{16} \text{ cm}^{-3}$  may not improve the cell efficiency and therefore, to get efficiencies above 7.5 %, other parameters have to be optimized.

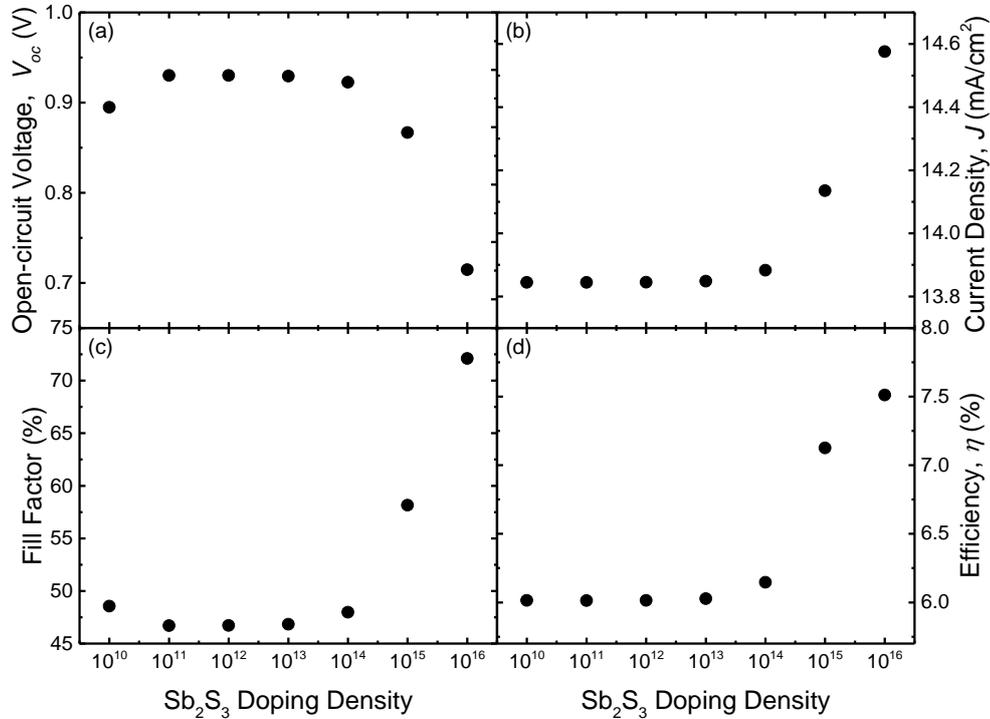


Figure 13 Variation in solar cell parameters with doping density of  $Sb_2S_3$ .

Finally, we considered all the optimum values obtained in sub-sections 3.1 – 3.6 (see Table 5) and obtained encouraging results of the  $V_{oc}$  of 750.8 mV,  $J_{sc}$  of  $15.23 \text{ mA}/\text{cm}^2$ , FF of 73.55% and PCE of 8.41% as shown in Table 6. These results show that  $Sb_2S_3$  solar cells with high efficiency can be achieved by optimizing the thickness and doping densities of both the  $TiO_2$  buffer layer and  $Sb_2S_3$  absorber layer, the electron affinity of  $TiO_2$  and more importantly the defects in  $Sb_2S_3$  which is the main challenge for  $Sb_2S_3$  absorber layer.

Table 5. Final optimized parameters of  $Sb_2S_3$  solar cell with  $TiO_2$  buffer layer

Parameter	Units	cp- $TiO_2$	$Sb_2S_3$
$X_e$ (Electron affinity)	eV	4.26	–
w (Thickness)	nm	50	140
Density of defects	$\text{cm}^{-3}$	No change	$1.0 \times 10^{15}$
$N_A$ (Carrier density of the acceptor)	$\text{cm}^{-3}$	–	$3.0 \times 10^{16}$
$N_D$ (Carrier density of the donor)	$\text{cm}^{-3}$	$1.0 \times 10^{17}$	–

Table 6. Results for optimized parameters of Sb<sub>2</sub>S<sub>3</sub> solar cell with TiO<sub>2</sub> buffer layer

	V <sub>oc</sub> (mV)	J <sub>sc</sub> (mA/cm <sup>2</sup> )	FF (%)	η (%)
Experiment [Choi <i>et al.</i> , 2014]	711	16.1	65	7.5
SCAPS Simulation (Start)	714.7	14.58	72.11	7.51
SCAPS Simulation (Final)	750.8	15.23	73.55	8.41

#### 4. Conclusions

Sb<sub>2</sub>S<sub>3</sub> solar cell performance is simulated and analyzed by the functions of the buffer layer and the absorber layer. The optimum thickness of the Sb<sub>2</sub>S<sub>3</sub> absorber layer and the TiO<sub>2</sub> buffer layer are found in the range of 130nm to 150nm and between 40nm and 50nm respectively. Increase in thickness of the buffer layer deteriorates the performance of the solar cell due to an increase in the length of electron pathways in TiO<sub>2</sub> and fewer photon penetration to the absorber layer. This leads to increase in recombination and electron back transfer reaction. Variation in doping density of buffer layer affects only the open circuit voltage while variations in defect density has no significant effect on the performance of the cell. Increasing the thickness of the Sb<sub>2</sub>S<sub>3</sub> absorber layer leads to increase in the short circuit current but with decrease in the open circuit voltage to a nearly constant 0.7 V due to increase in recombination kinetics at the interface and in the bulk of Sb<sub>2</sub>S<sub>3</sub>.

Increase in doping densities reduces the trap density in Sb<sub>2</sub>S<sub>3</sub> and therefore improves on charge collection from the absorber. These results can be used to obtain a highly improved thin film Sb<sub>2</sub>S<sub>3</sub> solar cell but there is need to optimize the fabrication process so as to achieve the above results.

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#### References

- [1] Abulikemu, M., S. D. Gobbo, D. H. Anjum, M. A. Malik, and O. M. Bakr, (2016) Colloidal Sb<sub>2</sub>S<sub>3</sub> nanocrystals: synthesis, characterization and fabrication of solid-state semiconductor sensitized solar cells: *Journal of Materials Chemistry A*, **4**(18): 6809–6814, doi:[10.1039/C5TA09546H](https://doi.org/10.1039/C5TA09546H).
- [2] Escorcia-García, J., D. Becerra, M. T. S. Nair, and P. K. Nair, (2014) Heterojunction CdS/Sb<sub>2</sub>S<sub>3</sub> solar cells using antimony sulfide thin films prepared by thermal evaporation: *Thin Solid Films*, **569**: 28–34, doi:[10.1016/j.tsf.2014.08.024](https://doi.org/10.1016/j.tsf.2014.08.024).
- [3] Sotelo Marquina, R. G., T. G. Sanchez, N. R. Mathews, and X. Mathew, (2017) Vacuum coated Sb<sub>2</sub>S<sub>3</sub> thin films: Thermal treatment and the evolution of its physical properties: *Materials Research Bulletin*, **90**: 285–294, doi:[10.1016/j.materresbull.2017.03.013](https://doi.org/10.1016/j.materresbull.2017.03.013).
- [4] Lakhdar, M. H., B. Ouni, and M. Amlouk, (2014) Thickness effect on the structural and optical constants of stibnite thin films prepared by sulfidation annealing of antimony films: *Optik*, **125** (10): 2295–2301, doi:[10.1016/j.ijleo.2013.10.114](https://doi.org/10.1016/j.ijleo.2013.10.114).

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- [5] Yuan, S., H. Deng, D. Dong, X. Yang, K. Qiao, C. Hu, Huaibing Song, Haisheng Song, Z. He, and J. Tang, (2016) Efficient planar antimony sulfide thin film photovoltaics with large grain and preferential growth: *Solar Energy Materials and Solar Cells*, **157**:887–893, doi:[10.1016/j.solmat.2016.07.050](https://doi.org/10.1016/j.solmat.2016.07.050).
- [6] Deng, H., S. Yuan, X. Yang, F. Cai, C. Hu, K. Qiao, J. Zhang, J. Tang, H. Song, and Z. He, (2017) Efficient and stable TiO<sub>2</sub>/Sb<sub>2</sub>S<sub>3</sub> planar solar cells from absorber crystallization and Se-atmosphere annealing: *Materials Today Energy*, **3**:15–23, doi:[10.1016/j.mtener.2017.02.001](https://doi.org/10.1016/j.mtener.2017.02.001).
- [7] Shaji, S., L. V. Garcia, S. L. Loreda, B. Krishnan, J. A. Aguilar Martinez, T. K. Das Roy, and D. A. Avellaneda, (2017) Antimony sulfide thin films prepared by laser assisted chemical bath deposition: *Applied Surface Science*, **393**:369–376, doi:[10.1016/j.apsusc.2016.10.051](https://doi.org/10.1016/j.apsusc.2016.10.051).
- [8] Ito, S., K. Tsujimoto, D.-C. Nguyen, K. Manabe, and H. Nishino, (2013) Doping effects in Sb<sub>2</sub>S<sub>3</sub> absorber for full-inorganic printed solar cells with 5.7% conversion efficiency: *International Journal of Hydrogen Energy*, **38**(36):16749–16754, doi:[10.1016/j.ijhydene.2013.02.069](https://doi.org/10.1016/j.ijhydene.2013.02.069).
- [9] Mushtaq, S., B. Ismail, M. Aurang Zeb, N. J. Suthan Kissinger, and A. Zeb, (2015) Low-temperature synthesis and characterization of Sn-doped Sb<sub>2</sub>S<sub>3</sub> thin film for solar cell applications: *Journal of Alloys and Compounds*, **632**:723–728, doi:[10.1016/j.jallcom.2015.01.307](https://doi.org/10.1016/j.jallcom.2015.01.307).
- [10] Darga, A., D. Mencaraglia, C. Longeaud, T. J. Savenije, B. O'Regan, S. Bourdais, T. Muto, B. Delatouche, and G. Dennler, (2013) On Charge Carrier Recombination in Sb<sub>2</sub>S<sub>3</sub> and Its Implication for the Performance of Solar Cells: *The Journal of Physical Chemistry C*, **117**(40):20525–20530, doi:[10.1021/jp4072394](https://doi.org/10.1021/jp4072394).
- [11] You, M. S., C.-S. Lim, D. H. Kwon, J. H. Heo, S. H. Im, and K. J. Chae, (2015) Oxide-free Sb<sub>2</sub>S<sub>3</sub> sensitized solar cells fabricated by spin and heat-treatment of Sb(III)(thioacetamide)<sub>2</sub>Cl<sub>3</sub>: *Organic Electronics*, **21**:155–159, doi:[10.1016/j.orgel.2015.02.015](https://doi.org/10.1016/j.orgel.2015.02.015).
- [12] Gao, C., M. Xu, B. K. Ng, L. Kang, L. Jiang, Y. Lai, and F. Liu, (2017) In situ growth of Sb<sub>2</sub>S<sub>3</sub> thin films by reactive sputtering on n-Si(100) substrates for top sub-cell of silicon based tandem solar cells: *Materials Letters*, v. 195, p. 186–189, doi:[10.1016/j.matlet.2017.02.046](https://doi.org/10.1016/j.matlet.2017.02.046).
- [13] Avilez Garcia, R. G., C. A. Meza Avendaño, M. Pal, F. Paraguay Delgado, and N. R. Mathews, (2016) Antimony sulfide (Sb<sub>2</sub>S<sub>3</sub>) thin films by pulse electrodeposition: Effect of thermal treatment on structural, optical and electrical properties: *Materials Science in Semiconductor Processing*, **44**:91–100, doi:[10.1016/j.mssp.2015.12.018](https://doi.org/10.1016/j.mssp.2015.12.018).
- [14] Gödel, K. C., Y. C. Choi, B. Roose, A. Sadhanala, H. J. Snaith, S. I. Seok, U. Steiner, and S. K. Pathak, 2015, Efficient room temperature aqueous Sb<sub>2</sub>S<sub>3</sub> synthesis for inorganic–organic sensitized solar cells with 5.1% efficiencies: *Chemical Communications*, **51**(41):8640–8643, doi:[10.1039/C5CC01966D](https://doi.org/10.1039/C5CC01966D).
- [15] Moon, S.-J., Y. Itzhaik, J.-H. Yum, S. M. Zakeeruddin, G. Hodes, and M. Grätzel, (2010) Sb<sub>2</sub>S<sub>3</sub>-Based Mesoscopic Solar Cell using an Organic Hole Conductor: *The Journal of Physical Chemistry Letters*, **1**(10):1524–1527, doi:[10.1021/jz100308q](https://doi.org/10.1021/jz100308q).
- [16] Choi, Y. C., D. U. Lee, J. H. Noh, E. K. Kim, and S. I. Seok, (2014) Highly Improved Sb<sub>2</sub>S<sub>3</sub> Sensitized-Inorganic–Organic Heterojunction Solar Cells and Quantification of Traps by Deep-Level Transient Spectroscopy: *Advanced Functional Materials*, **24**(23):3587–3592, doi:[10.1002/adfm.201304238](https://doi.org/10.1002/adfm.201304238).
- [17] Du, H.-J., W.-C. Wang, and J.-Z. Zhu, (2016) Device simulation of lead-free CH<sub>3</sub>NH<sub>3</sub>SnI<sub>3</sub> perovskite solar cells with high efficiency: *Chinese Physics B*, **25**(10):108802, doi:[10.1088/1674-1056/25/10/108802](https://doi.org/10.1088/1674-1056/25/10/108802).
- [18] Khoshsirat, N., and N. A. M. Yunus, (2013) Numerical simulation of CIGS thin film solar cells using SCAPS-1D, *in* 2013 IEEE Conference on Sustainable Utilization and Development in Engineering and Technology (CSUDET): 63–67, doi:[10.1109/CSUDET.2013.6670987](https://doi.org/10.1109/CSUDET.2013.6670987).
- [19] Burgelman, M., P. Nollet, and S. Degraeve, (2000) Modelling polycrystalline semiconductor solar cells: *Thin Solid Films*, **361–362**:527–532, doi:[10.1016/S0040-6090\(99\)00825-1](https://doi.org/10.1016/S0040-6090(99)00825-1).

- [20] Ben Nasr, T., H. Maghraoui-Meherzi, H. Ben Abdallah, and R. Bennaceur, (2011) Electronic structure and optical properties of Sb<sub>2</sub>S<sub>3</sub> crystal: *Physica B: Condensed Matter*, **406**(2):287–292, doi:[10.1016/j.physb.2010.10.070](https://doi.org/10.1016/j.physb.2010.10.070).
- [21] Tumelero, M. A., R. Faccio, and A. A. Pasa, (2016) Unraveling the Native Conduction of Trichalcogenides and Its Ideal Band Alignment for New Photovoltaic Interfaces: *The Journal of Physical Chemistry C*, **120**(3):1390–1399, doi:[10.1021/acs.jpcc.5b10233](https://doi.org/10.1021/acs.jpcc.5b10233).
- [22] Lee, D. U., S. Woo Pak, S. Gook Cho, E. Kyu Kim, and S. Il Seok, (2013) Defect states in hybrid solar cells consisting of Sb<sub>2</sub>S<sub>3</sub> quantum dots and TiO<sub>2</sub> nanoparticles: *Applied Physics Letters*, **103**(2):023901, doi:[10.1063/1.4813272](https://doi.org/10.1063/1.4813272).
- [23] Mostefaoui, M., H. Mazari, S. Khelifi, A. Bouraiou, and R. Dabou, (2015) Simulation of High Efficiency CIGS Solar Cells with SCAPS-1D Software: *Energy Procedia*, **74**:736–744, doi:[10.1016/j.egypro.2015.07.809](https://doi.org/10.1016/j.egypro.2015.07.809).
- [24] Roy, B., B. R. Chakraborty, R. Bhattacharya, and A. K. Dutta, (1978) Electrical and magnetic properties of antimony sulphide (Sb<sub>2</sub>S<sub>3</sub>) crystals and the mechanism of carrier transport in it: *Solid State Communications*, **25**(11):937–940, doi:[10.1016/0038-1098\(78\)90306-X](https://doi.org/10.1016/0038-1098(78)90306-X).