Performance evaluation of Sb2Se3-based solar photovoltaic cells with various ETL and Cu2O as HTL by SCAPS-1D

Abdelmajid El Khalfi  
LM3ER-OTEA Department of Physics, Faculty of Sciences and Techniques, BP 509 Boutalamine 52000, Errachidia, Moulay Ismail University of Meknes, Morocco, elkhalfi-abdelmajid@hotmail.fr

Lhoussayne Et-taya  
LM3ER-OTEA Department of Physics, Faculty of Sciences and Techniques, BP 509 Boutalamine 52000, Errachidia, Moulay Ismail University of Meknes, Morocco

Youssef Achenani  
LM3ER-OTEA Department of Physics, Faculty of Sciences and Techniques, BP 509 Boutalamine 52000, Errachidia, Moulay Ismail University of Meknes, Morocco

Mustapha Sahal  
ERMAM, Ouarzazate Polydisciplinary Faculty, University of Ibn Zohr, 45000, Agadir, Morocco

Lahoucine Elmaimouni  
ERMAM, Ouarzazate Polydisciplinary Faculty, University of Ibn Zohr, 45000, Agadir, Morocco

See next page for additional authors

Follow this and additional works at: https://kijoms.uokerbala.edu.iq/home

Recommended Citation  
El Khalfi, Abdelmajid; Et-taya, Lhoussayne; Achenani, Youssef; Sahal, Mustapha; Elmaimouni, Lahoucine; and Benami, Abdellah (2023) "Performance evaluation of Sb2Se3-based solar photovoltaic cells with various ETL and Cu2O as HTL by SCAPS-1D," Karbala International Journal of Modern Science: Vol. 9 : Iss. 3 , Article 3. Available at: https://doi.org/10.33640/2405-609X.3303

This Research Paper is brought to you for free and open access by Karbala International Journal of Modern Science. It has been accepted for inclusion in Karbala International Journal of Modern Science by an authorized editor of Karbala International Journal of Modern Science. For more information, please contact abdulateef1962@gmail.com.
Performance evaluation of Sb2Se3-based solar photovoltaic cells with various ETL and Cu2O as HTL by SCAPS-1D

Abstract
Sb2Se3 photovoltaic cells have garnered much attention recently because of their inexpensive manufacture and long-term stability. So, different buffer layers were investigated using the SCAPS software to improve the device's output. By comparing J-V characteristics and QE for cells with different ETLs, WS2 was discovered to be the best ETL. The impact of carrier concentrations, the active layer, ETL and HTL thickness, absorber density of defects, and electron affinity were also investigated. It was discovered that WS2 could be a good substitute for conventional ETLs. After optimization, efficiency is 30.03%, FF is 87.13%, JSC is 37.15 mA/cm², and VOC is 0.928 V. This research provides a new strategy to fabricate high-efficiency and Cd-free Sb2Se3-based photovoltaic cells.

Keywords
Sb2Se3 solar cells; WS2 ETL; Cu2O HTL; scaps-1D

Creative Commons License
This work is licensed under a Creative Commons Attribution-Noncommercial-No Derivative Works 4.0 License.

Authors
Abdelmajid El Khalfi, Lhoussayne Et-taya, Youssef Achenani, Mustapha Sahal, Lahoucine Elmaimouni, and Abdellah Benami

This research paper is available in Karbala International Journal of Modern Science: https://kijoms.uokerbala.edu.iq/home/vol9/iss3/3
RESEARCH PAPER

Performance Evaluation of $\text{Sb}_2\text{Se}_3$-based Solar Photovoltaic Cells with Various ETL and Cu$_2$O as HTL by SCAPS-1D

Abdelmajid El Khalfi $^a$, Lhoussayne Et-tayaa $^a$, Youssef Achenani $^a$, Mustapha Sahal $^b$, Lahoucine Elmaimouni $^b$, Abdellah Benami $^{a,**}$

$^a$ LM3ER-OTEA Department of Physics, Faculty of Sciences and Techniques, BP 509 Boutalamine, 52000, Errachidia, Moulay Ismail University of Meknes, Morocco
$^b$ ERMAM, Ouarzazate Polydisciplinary Faculty, University of Ibn Zohr, 45000, Agadir, Morocco

Abstract

Sb$_2$Se$_3$ photovoltaic cells have garnered much attention recently because of their inexpensive manufacture and long-term stability. So, different buffer layers were investigated using the SCAPS software to improve the device's output. By comparing J-V characteristics and QE for cells with different ETLs, WS$_2$ was discovered to be the best ETL. The impact of carrier concentrations, the active layer, ETL and HTL thickness, absorber density of defects, and electron affinity were also investigated. It was discovered that WS$_2$ could be a good substitute for conventional ETLs. After optimization, efficiency is 30.03%, FF is 87.13%, J$_{SC}$ is 37.15 mA/cm$^2$, and V$_{OC}$ is 0.928 V. This research provides a new strategy to fabricate high-efficiency and Cd-free Sb$_2$Se$_3$-based photovoltaic cells.

Keywords: Sb$_2$Se$_3$ solar cells, WS$_2$ ETL, Cu$_2$O HTL, SCAPS-1D

1. Introduction

Energy needs are growing at a very fast rate because the population is growing quickly and people are using more energy per person [1]. Fossil fuels provide enough energy to meet current needs but are used up and running out. Several researchers advocate for the use of renewable energy sources.

Electricity as an energy carrier is obtained from photovoltaic (PV) cells by converting the energy carried by light rays into electricity. Four generations of PV cells exist, which differ in the absorbent material utilized [2]. The second generation, also called thin-film solar cells, includes, among other thin-film technologies, copper-indium-gallium-diselenide, and cadmium-telluride, which have been extensively studied and have reached very high power conversion efficiencies (PCE) of around 22.1 and 23.3%, respectively [3]. Nevertheless, the expensive cost of Ge, Te, and In, along with the toxicity of Cd, may prevent their widespread use [4]. As a result, earth-abundant, inexpensive, and non-toxic PV materials have attracted much attention in recent decades [5]. In this context, Sb$_2$Se$_3$ can be a fascinating material used as the active layer in a PV cell. This compound has an orthogonal crystal structure and is a p-type semiconductor [6]. It is a more robust PV absorber because of its extremely high absorption coefficient at lower wavelengths ($>10^{5}$ cm$^{-1}$) [7]. It has a direct bandgap of 1.1–1.3 eV [8] and excellent mobility of holes of 42 cm$^2$ V$^{-1}$s$^{-1}$ [9].

Several growth techniques for depositing Sb$_2$Se$_3$ thin films and fabricating solar cells with different power conversion efficiencies have been investigated. A chemical bath deposition (CBD) was used by Messina et al. to prepare Sb$_2$Se$_3$ with a PCE of 0.66% in 2009 [10]. Six years later, Zhou et al. [11] used rapid thermal evaporation (RTE) to achieve a PCE of 5.6%. Wen et al. employed the method of
vapor transport deposition (VTD) in 2018, and the PCE was increased to 7.6% [12]. Duan et al. achieved the highest conversion efficiency, exceeding 10% in 2022, using the close-spaced sublimation (CSS) technique [13].

The output of the thin-film PV cell is influenced by the photoelectric properties of the various layers that make up the cell. One of these layers is the electron transport layer (ETL), which ensures the transport and collection of photo-generated electrons. The most common ETL is the CdS layer [14]. However, CdS has some drawbacks, including i) diffusion of Cd\(^{2+}\) from the buffer layer, which leads to low stability under illumination [15], ii) high toxicity of Cd, and iii) blue light is significantly absorbed by CdS, which results in a low harvest of light-generated carriers due to the high defect density in the CdS layer. To enhance the performance of solar cells using a Sb\(_2\)Se\(_3\) absorption layer, an analysis of ETL is necessary. As a result, we use a numerical simulation to assess the efficiency of the FTO/ETL/Sb\(_2\)Se\(_3\)/Cu\(_2\)O/Au arrangement with various ETLs, such as WS\(_2\), SnO\(_2\), TiO\(_2\), CdS, WO\(_3\), and SnS\(_2\), by examining the impact of parameters such as the thickness of the Sb\(_2\)Se\(_3\) and different buffer layers, defect density, doping concentration of the active layer and WS\(_2\) buffer layers, HTL, and electron affinity on the output characteristics of the PV device using the SCAPS-1D program.

2. Materials and methods

Fig. 1 depicts the arrangement of the device in our modeling experiment, which is FTO/ETL/Sb\(_2\)Se\(_3\)/Cu\(_2\)O/Au. The studied device consists of a back contact in Au, which collects the holes (positive charge carriers), cuprous oxide (Cu\(_2\)O) as the HTL, and the p-Sb\(_2\)Se\(_3\) active layer in which electron–hole pairs are generated. Then, WS\(_2\), SnO\(_2\), TiO\(_2\), CdS, WO\(_3\), and SnS\(_2\) are used as an ETL. After that, the ETL is then stacked with FTO (SnO\(_2\): F), which acts as a TCO collecting electrons.

In this work, we used the SCAPS-1D program developed by the University of Gent, Belgium [16]. It is fast, interactive, flexible, free for PV research, and may offer a good match between simulation and experiment outputs. Then it can perform simulations of many popular measures: C\(_V\), C\(_f\), I\(_V\), and QE. Three fundamental equations serve as the foundation for theoretical computations, and they are as follows:

\[
\frac{\partial^2 \psi}{\partial x^2} = -\frac{q}{\epsilon} \left[ p(x) - n(x) + N_D - N_A + \rho_p - \rho_n \right] \tag{1}
\]

where \(\psi\) is the dielectric constant of the semiconductor material, \(q\) is the electron charge, \(\psi\) is the electrostatic potential, \(N_D, N_A\) is the density of donor-like (acceptor-like), \(n, p\) is electron (hole) concentration, \(\rho_n, \rho_p\) is electron (hole) distribution, and \(x\) is the position.

Given are the hole and electron continuity equations:

\[
\frac{dJ_p}{dx} = q(G - R) \tag{2}
\]

\[
\frac{dJ_n}{dx} = -q(G - R) \tag{3}
\]

where \(R\) is carrier recombination rate, \(G\) is carrier generation rate, \(J_p\) is hole current density, and \(J_n\) is electron current density.

The drift-diffusion equation for electrons and holes:

\[
J_n = qD_n \frac{\partial n}{\partial x} - q\mu_n \psi \frac{\partial \psi}{\partial x} \tag{4}
\]

\[
J_p = -qD_p \frac{\partial p}{\partial x} - q\mu_p \psi \frac{\partial \psi}{\partial x} \tag{5}
\]

where \(D_n\) and \(D_p\) are the electron and hole diffusion coefficients, respectively, and \(\mu_p, \mu_n\) are hole and electron mobility.

The following values and parameters employed in the calculation are selected from the literature [17–20] and are listed in Table 1. The front and back contact work functions are 4.4 eV (FTO) and 5.1 eV (Au). The surface recombination rates of holes and electrons are fixed at \(10^7\) cm/s. The working temperature is set at 300 K, and the standard AM1.5G spectrum with an incident power density of 1000 W/m\(^2\) is used for all simulations.

The defect for different layer materials is fixed at the neutral gaussian type distribution, having a
characteristic value of 0.1 eV; ETL and HTL interfaces defects are at the middle of the interface gap with a defect density \( N_0 \) of \( 10^{15} \text{ cm}^{-3} \), and the electron and hole capture cross-section are both set as \( 10^{-19} \text{ cm}^2 \). The optical absorption for all layers was obtained using the following equation:

\[
\alpha(h\lambda) = \left( \frac{\alpha_0 + \beta_0 E_g}{h\lambda} \right) \left( \frac{h\lambda}{E_g} - 1 \right)
\]

where \( \alpha_0 = 10^{-12} \text{ cm}^{-1} \) and \( \alpha_0 = 10^5 \text{ cm}^{-1} \).

3. Results and discussion

3.1. Alternative buffer layer to the CdS

3.1.1. J-V and EQE characteristics

In PV systems, ETLs combine with the absorber to create a p-n junction and extract photogenerated electrons to the front electrode. Because a suitable and non-toxic ETL is required for Sb\(_2\)Se\(_3\)-based PV material, numerical simulation was done to evaluate the impact of various buffer layers on the key characteristics of PV cells. One of the more widely used buffer layers in solar cells is CdS. However, it contains the harmful Cd element, which has a narrow bandgap, and processing at higher temperatures causes intermixing. Fig. 2 depicts the comparison of J-V characteristics (a) and EQE (b) among different ETLs (WS\(_2\), CdS, SnS\(_2\), WO\(_3\), SnO\(_2\), TiO\(_2\)), and Table 2 summarizes the output performances. Fig. 2 (a) shows that the three layers WS\(_2\), SnO\(_2\), and TiO\(_2\) performed better than the standard layer CdS, as confirmed by the inset of Fig. 2 (a). The highest PCE of 24.98% is achieved from the device cell using WS\(_2\) as ETL. The bandgap alignment and conduction band offset at the ETL/Sb\(_2\)Se\(_3\) interface can be used to explain these results. It was also found that the cell with WS\(_2\), \( J_{sc} \), and \( V_{oc} \) has the most excellent mobility among all ETLs, which could be attributed to better carrier mobility.

The quantum efficiency of the solar cell is defined as the ratio of the number of carriers collected by the device to the number of incident photons. The \( J_{sc} \) and EQE were observed to be directly proportional to each other, as given by equation (7) [21].

\[
\text{EQE}(\lambda) = \frac{h \cdot c \cdot J_{sc}}{q \cdot \lambda \cdot I_0(\lambda)}
\]

Whereby, \( h, c, J_{sc}, q, \lambda, \) and \( I_0(\lambda) \) are Plank’s constant, light velocity, short-circuit current, electron charge, the wavelength of exciter light, and the electric current due to the photoelectric effect, respectively.

Fig. 2(b) shows the EQE curves of the structure Cu\(_2\)O/Sb\(_2\)Se\(_3\)/ETL/FTO as a function of wavelength for various ETLs in the 200–1100 nm wavelength range. With a maximum absorption of more than 90% in the visible region, the EQE has demonstrated a similar trend for all ETLs.

As can be seen, the curve exhibits an increased response in the region between 200 and 350 nm, where SnS\(_2\)-based solar cells have the most remarkable capacity for sunlight absorption. After 350 nm, it is nearly constant up to 600 nm, and then it gradually decreases until it reaches zero at the wavelength ~1050 nm, which may be due to no light being absorbed below the bandgap. Furthermore, the WS\(_2\) buffer layer absorbs the most solar light in the visible region. The WS\(_2\)-based PV device is the most efficient for solar light absorption among all other ETL-based solar cells because frequent solar radiation is in the visible area.

3.1.2. Energy band diagram

Band alignment significantly impacts the carrier transport across the heterojunction and thus on the performance of the solar cells. Under equilibrium

Table 1. Settings used in the simulation.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Cu(_2)O</th>
<th>Sb(_2)Se(_3)</th>
<th>WS(_2)</th>
<th>CdS</th>
<th>SnS(_2)</th>
<th>WO(_3)</th>
<th>SnO(_2)</th>
<th>TiO(_2)</th>
<th>FTO</th>
</tr>
</thead>
<tbody>
<tr>
<td>( W (\mu m) )</td>
<td>0.1</td>
<td>0.5</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
<td>0.25</td>
</tr>
<tr>
<td>( E_g (eV) )</td>
<td>2.1</td>
<td>1.2</td>
<td>1.8</td>
<td>2.4</td>
<td>2.24</td>
<td>2.6</td>
<td>2.6</td>
<td>2.6</td>
<td>3.2</td>
</tr>
<tr>
<td>( \chi (eV) )</td>
<td>3.2</td>
<td>4.04</td>
<td>3.95</td>
<td>4</td>
<td>4.24</td>
<td>3.8</td>
<td>3.8</td>
<td>3.8</td>
<td>4</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>7.11</td>
<td>18</td>
<td>13.6</td>
<td>9</td>
<td>10</td>
<td>4.8</td>
<td>4.8</td>
<td>4.8</td>
<td>9</td>
</tr>
<tr>
<td>( N_{c}(cm^{-3}) )</td>
<td>( 2.2 \times 10^{20} )</td>
<td>( 2.2 \times 10^{18} )</td>
<td>( 2.2 \times 10^{18} )</td>
<td>( 2.2 \times 10^{19} )</td>
<td>( 2.2 \times 10^{18} )</td>
<td>( 2.2 \times 10^{21} )</td>
<td>( 2.2 \times 10^{18} )</td>
<td>( 2.2 \times 10^{18} )</td>
<td>( 10 \times 10^{21} )</td>
</tr>
<tr>
<td>( N_{v}(cm^{-3}) )</td>
<td>( 5.5 \times 10^{19} )</td>
<td>( 1.8 \times 10^{18} )</td>
<td>( 1.8 \times 10^{19} )</td>
<td>( 1.8 \times 10^{18} )</td>
<td>( 1.8 \times 10^{19} )</td>
<td>( 2.2 \times 10^{21} )</td>
<td>( 2.2 \times 10^{19} )</td>
<td>( 2.2 \times 10^{19} )</td>
<td>( 2.0 \times 10^{20} )</td>
</tr>
<tr>
<td>( V_{c}(cm/s) )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
</tr>
<tr>
<td>( V_{p}(cm/s) )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
<td>( 10^7 )</td>
</tr>
<tr>
<td>( \mu_{c}(cm^2/Vs) )</td>
<td>3.4</td>
<td>15</td>
<td>100</td>
<td>100</td>
<td>50</td>
<td>30</td>
<td>100</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>( \mu_{p}(cm^2/Vs) )</td>
<td>3.4</td>
<td>5.1</td>
<td>100</td>
<td>25</td>
<td>50</td>
<td>30</td>
<td>25</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>( N_{D}(cm^{-3}) )</td>
<td>0</td>
<td>0</td>
<td>10^{18}</td>
<td>10^{18}</td>
<td>10^{17}</td>
<td>6.35 \times 10^{17}</td>
<td>10^{18}</td>
<td>10^{16}</td>
<td>10^{18}</td>
</tr>
<tr>
<td>( N_{A}(cm^{-3}) )</td>
<td>10^{18}</td>
<td>10^{17}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( N_{i}(cm^{-3}) )</td>
<td>10^{15}</td>
<td>10^{15}</td>
<td>10^{15}</td>
<td>10^{15}</td>
<td>10^{15}</td>
<td>10^{15}</td>
<td>10^{15}</td>
<td>10^{15}</td>
<td>10^{15}</td>
</tr>
</tbody>
</table>
conditions, the band diagram of the Sb$_2$Se$_3$ solar cell with different ETLs under light is shown in Fig. 3.

The difference in band gap and electronic affinities between the different layers of the solar cell generates a conduction band offset (CBO) $\Delta E_c$, and a valence band offset (VBO) $\Delta E_v$, at the interface. To determine these offset values, SCAPS-1D uses Anderson’s model [22]:

$$
\Delta E_c = \chi_{\text{absorber}} - \chi_{\text{ETL}}
$$

(8)

$$
\Delta E_v = \Delta E_g + \Delta E_c
$$

(9)

According to the values of the electron affinity of the ETL and that of the absorbing layer, the energy cliff is obtained with a negative CBO, and the energy spike is obtained with a positive CBO. A high-efficiency solar cell requires a $0.0 - 0.4$ eV conduction band offset. As shown in Fig. 3, the WS$_2$ buffer layer produces a positive CBO value of 0.09 eV, whereas the CdS, TiO$_2$, and SnO$_2$ ETLs produce the same positive CBO value of 0.04 eV WS$_2$ has the highest CBO, resulting in a high barrier (or spike) at the WS$_2$/Sb$_2$Se$_3$ interface. Creating a spike-like structure works as band bending to decrease recombination and facilitate the separation of charge carriers. As a result, the open circuit voltage and fill factor have increased values, which improve the solar cell’s performance.

### 3.2. Optimization of the thickness of the Sb$_2$Se$_3$

Throughout this part, while maintaining other variables constant, we looked at how active layer thickness affected output cells for various ETLs in the range of 0.1–3 $\mu$m, as shown in Table 1. The variance in absorber layer thickness impacts the carrier diffusion length. The thinner the absorbing layer, the slower the absorption rate, reducing the $J_{sc}$ and yield. Similarly, increasing the active layer’s thickness prevents charge carriers from flowing to the charge collection layers, resulting in a drop in efficiency [23]. Fig. 4 demonstrates that the output metrics increase rapidly as the thickness of the absorbing layer increases but afterward decline very softly. Fig. 4 also shows that WS$_2$ is the best-performing buffer layer across the whole range of absorber layer thicknesses, with the FTO/WS$_2$/Sb$_2$Se$_3$/Cu$_2$O/Au PV device at a thickness of 1 $\mu$m having the most excellent output, with PCE an of 25.88%, a $J_{sc}$ of 37.73 mA/cm$^2$, a $V_{oc}$ of 0.82 V, and a FF of 83.36%. According to the simulation results, WS$_2$ can be a good substitute for the traditional CdS buffer layer since it has excellent conductivity and high carrier mobility, which leads to higher $J_{sc}$ and PCE [24,25].

### 3.3. Optimization of the thickness of the WS$_2$ buffer layer

The buffer layer’s thickness is critical to optimizing the performance of PV devices. Since a thicker layer absorbs more photons than a thinner layer, fewer photons reach the absorbent layer, leading to high photon loss and a decrease in the quantum efficiency of the solar cell, so the buffer layer’s thickness must be lower than the absorber layer’s for electrons to be quickly collected at the
Fig. 5(a–d) illustrates the influence of WS2 thickness on the basic parameters of Se2Sb3-based solar cells while keeping the thickness of the Se2Sb3, FTO, and Cu2O layers constant at 1 μm, 0.25 μm and 0.1 μm, respectively. The JSC rises considerably as the thickness of the absorption layer increases from 50 nm to 375 nm and then gradually decreases after 375 nm, as illustrated in Fig. 5 (b). The highest value of JSC is 36.04 mA/cm² at 375 nm thickness. While the VOC varies very slightly, it keeps almost the exact value of 0.834 V as the thickness of the buffer layer increases further.

We can observe from Fig. 5 (d) that the increase in WS2 thickness induces a slight increase in efficiency from 24.98% to 25.062% for thicknesses of 50 and 450 nm, respectively. The PCE increases and reaches a maximum value of 25.065% at 400 nm and then decreases slowly due to the absorption of some photons in the thick buffer layer. A too-thick buffer layer can also result in a low carrier separation rate [27].

3.4. Optimization of a carrier concentration of Sb2Se3 absorber layer and WS2 ETL

The doping concentration (N_A) of the Sb2Se3 absorber layer has a significant effect on solar cell outputs. All other parameters are held constant while the N_A is changed from 10^{12} cm^{-3} to 10^{19} cm^{-3} keeping. Fig. 6 depicts the impact of shallow acceptor density on various cell parameters. Properties of solar cells like VOC, FF, and PCE follow a similar pattern as acceptor concentration density rises. These three parameters are slightly enhanced as the concentration increases from 10^{12} cm^{-3} to 10^{14} cm^{-3} and increases linearly after 10^{14} cm^{-3}. At 10^{19} cm^{-3}, VOC, FF, and PCE reached values of 0.911 V, 86.59%, and 28.91%, respectively. The potential integrated with the solar cell junction increases as the acceptor density in the absorber layer rises, requiring the charge carriers to move toward the corresponding electrodes and enhancing photoinduced carrier collection and cell efficiency [28]. The JSC slowly increases with increasing N_A from 10^{12} - 10^{16} cm^{-3}. JSC decreases with increasing N_A beyond 10^{16} cm^{-3}. Increased concentration in the absorption layer causes increased diffusion and hence, reduced mobility, lifetime, and diffusion length, resulting in a diminution of JSC. As a result, increased concentrations lead to a higher probability of recombination at the back surface [1].

The influence of doping concentration in the WS2 ETL layer on the output is examined by varying the
values of $N_D$ in the range of $10^{12}$–$10^{19}$ cm$^{-3}$ while maintaining $N_A$ for the absorber at $10^{19}$ cm$^{-3}$. The four parameters (efficiency, $V_{OC}$, FF, and $J_{SC}$) are presented in Fig. 7. When the concentration increases from $10^{12}$ to $10^{17}$ cm$^{-3}$, PCE and FF gradually increase until they reach their optimal value at $10^{17}$ cm$^{-3}$, at which point they significantly decrease. $V_{OC}$ decreases slightly until $10^{17}$ cm$^{-3}$, then the decrease becomes abrupt. On the other hand, the value of $J_{SC}$ begins to rise slowly between $10^{12}$ cm$^{-3}$ to $10^{15}$ cm$^{-3}$, then rises sharply between $10^{15}$ cm$^{-3}$ and $10^{19}$ cm$^{-3}$. This trend might be explained by a decrease in the space charge area brought on by a greater doping concentration [29]. The performance parameters’ optimal values are $PCE = 29.25\%$, $J_{SC} = 36.51$ mA cm$^{-2}$, $FF = 86.75\%$ and $V_{OC} = 0.924$ V, which are obtained at $10^{17}$ cm$^{-3}$.

3.5. Optimization of Cu$_2$O HTL thickness and carrier concentration

Cu$_2$O’s significant role as an HTL is to collect and transmit photogenerated holes to the back electrode. Moreover, it blocks electrons and promotes their transport to the front electrode while reflecting photons to the absorption layer, increasing the charge carrier concentration and decreasing recombination in the back layer, making the connection more ohmic and increasing photocurrent [30]. Fig. 8 depicts the impact of hole transport layer thickness on output parameters depending on doping concentration. The thickness and
concentration of HTL were changed from 5 nm to 50 nm and from \(10^{12}\) cm\(^{-3}\) to \(10^{19}\) cm\(^{-3}\), respectively. As the HTL layer thickness grows, all electrical properties increase similarly. Except for \(V_{OC}\), which can be constant, \(J_{SC}\), FF, and PCE increase weakly and become constant at 30 nm thickness.

Regarding how the quantity of HTL carriers affects the efficiency of solar cells. The electrical parameter is constant between \(10^{12}\) and \(10^{17}\) cm\(^{-3}\) but improves significantly above \(10^{19}\) cm\(^{-3}\). PCE achieved a value of 29.61\% at a thickness of 30 nm and a concentration of \(10^{19}\) cm\(^{-3}\). \(J_{SC}\), \(V_{OC}\), and FF reached the values of 36.77 mA/cm\(^2\), 0.926 V, and 86.96\%, respectively. A very high electric field generated at the interface of Cu\(_2\)O/Sb\(_2\)Se\(_3\) by an intense carrier concentration slows the flow of minority electrons toward the interface, reducing interface recombination and enhancing cell performance [28].

3.6. Optimization of electron affinities of ETL and HTL

The electron affinities of ETL and HTL are critical in determining the band offset between ETL and the absorption layer and between HTL and the absorption layer, which is a determinant in carrier recombination at the interface and is used to calculate \(V_{OC}\) [31]. Fig. 9 depicts the PCE, \(V_{OC}\), \(J_{SC}\), and FF fluctuation as a function of WS\(_2\) ETL and Cu\(_2\)O HTL electron affinity. When the electron affinity of the ETL layer is adjusted from 3.8 eV to 4.2 eV, the values of \(J_{SC}\) increase dramatically from 3.8 to 4 eV and then become practically saturated when the electron affinity is raised over 4 eV. When the electron affinity of ETL increased from 3.8 to 4 eV, the \(V_{OC}\), FF, and efficiency increased but then decreased as the electron affinity increased further.

To achieve the best conversion efficiency of the Sb\(_2\)Se\(_3\) solar cell, the electron affinity value of 4 eV for the WS\(_2\) as an ETL is used.

Fig. 9 shows, on the other hand, that the effect of HTL electron affinity (increased from 3 eV to 3.5 eV) on PV cell performance is minor compared to the impact of ETL electron affinity. The performance parameters gradually improve with increasing electron affinity and become nearly constant at 3.4 eV. After optimizing the electron affinity values of ETL and HTL at 4 eV and 3.4 eV, respectively, the PCE of 30.03\%, the \(J_{SC}\) of 37.15 mA cm\(^{-2}\), FF of 87.13\% and the \(V_{OC}\) of 0.928 V were obtained. The bandgap offset is reduced by optimal electron affinities, enabling improved energy alignment and charge transfer between active and transport layers [32].

3.7. Influence of the defect density of the absorber and WS\(_2\)

The optoelectronic properties of the materials may change as a result of defects in the material system. Higher levels of a defect in the absorbent layer lead to higher recombination due to pinhole formation, increased film degradation, reduced stability, and worse overall device performance [33]. The influence of Sb\(_2\)Se\(_3\) defect density and ETL defect density on PV system output is shown in Fig. 10. For both layers, the defect density \(N_t\) ranges from \(10^{12}\) cm\(^{-3}\) to \(10^{19}\) cm\(^{-3}\). Once the absorber defect density is less than \(10^{14}\) cm\(^{-3}\), the device’s effectiveness is unaffected mainly, with PCE getting close to 31\%. With increasing defect state density, all parameters decrease above this value. To improve efficiency, Sb\(_2\)Se\(_3\) defects should be reduced to \(10^{14}\) cm\(^{-3}\). As a result, a rise in defects indicates a decrease in charge...
carrier diffusion length and the appearance of carrier recombination in the active layer, which directly reduces PCE [34].

In terms of ETL defect density, it has increased from $10^{12}$ to $10^{19}$ cm$^{-3}$. All parameters remain nearly constant until the defect density of $10^{16}$ cm$^{-3}$ drops dramatically. $V_{OC}$ does not change significantly and almost maintains its value of 0.928 V. Furthermore, as illustrated in Fig. 10, defects in the active layer negatively affect cell performance compared to defects in the WS$_2$ layer.

4. Comparative study

After optimizing the interesting parameters of our proposed solar cell, such as thickness, carrier concentration, and defect density of the ETL, HTL, and absorber, the results of the PV parameters are $J_{SC} = 37.15$ mA/cm$^2$, $V_{OC} = 0.928$ V, FF = 87.13%, and PCE = 30.03%. The initial cell had the following performance values: $J_{SC} = 35.95$ mA/cm$^2$, $V_{OC} = 0.834$ V, FF = 83.28%, and PCE = 24.98%. We can conclude that there is an increase in power conversion efficiency of
Fig. 9. Contour graphs of PV cell outputs depending on the electron affinity of WS₂ ETL and CuO₂ HTL.

Fig. 10. Output parameters variation vs the defect density of the absorber and WS₂.
about 20%. The optimized J–V characteristics and the quantum efficiency as a function of the wavelength are presented in Fig. 11 (a) and (b), respectively. In addition, the comparison between the simulated module and some literature results of simulating the Sb$_2$Se$_3$-based solar cell is listed in Table 3. This paper shows that the WS$_2$ material can serve as a buffer layer and replace the conventional CdS layer. It must be processed, and further experimental studies are needed to improve efficiency.

### 5. Conclusion

In this work, Antimony Selenide PV cells with a design of FTO/ETL/Sb$_2$Se$_3$/Cu$_2$O/Au were numerically simulated and optimized using the SCAPS-1D program. To compare ETL layers, we employed several buffer layers (WS$_2$, CdS, TiO$_2$, SnO$_2$, WO$_3$, and SnS$_2$), and WS$_2$ was the best candidate as a buffer layer to replace standard CdS buffer layers. The PV performance of the modeled device with various thicknesses and doping concentrations of Sb$_2$Se$_3$, WS$_2$, and Cu$_2$O has been analyzed to optimize the time and cost of Sb$_2$Se$_3$ solar cells. The optimal absorber layer, WS$_2$ layer, and Cu$_2$O layer thicknesses are 1000 nm, 300 nm, and 40 nm, with carrier concentrations of $10^{19}$, $10^{17}$, and $10^{19}$ cm$^{-3}$, respectively. The electron affinity of WS$_2$ and Cu$_2$O has been optimized, yielding values of 4 eV and 3.4 eV, respectively. The defect density in the absorber and WS$_2$ should be less than $10^{14}$ cm$^{-3}$ and $10^{16}$ cm$^{-3}$, respectively. The final optimized device has a PCE of 30.03%, an FF of 87.13%, a $J_{SC}$ of 37.15 mA/cm$^2$, and a $V_{OC}$ of 0.928 V.

### Conflict of interest

The authors declare that there are no conflicts of interest.

### Acknowledgments

The authors thank Dr. Marc Burgelman from Ghent University Belgium for providing the SCAPS simulator.

### References

[1] T. Ouslimane, L. Et-taya, L. Elmaimouni, A. Benami, Impact of absorber layer thickness, defect density, and operating


[24] L. Et-taya, T. Oussilane, A. Benami, Numerical analysis of earth-abundant Cu2ZnSn(SxSe1-x)4 solar cells based on


