Simulation of the Sb$_2$Se$_3$ solar cell with a hole transport layer

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Abstract
A model of the Sb$_2$Se$_3$ solar cell with a hole transport layer (HTL) has been investigated by solar cell capacitance simulator (SCAPS). The influence of different HTLs on device performance has been firstly analyzed, and CuO has been found to be the best HTL. Then, Sb$_2$Se$_3$ thickness, CuO thickness, the doping concentration of CuO, the hole mobility of CuO, the defect density of Sb$_2$Se$_3$ layer, the defect density at the CdS/Sb$_2$Se$_3$ interface, and the work function of metal electrode on device performance have been systematically studied. The optimum thicknesses of Sb$_2$Se$_3$ and CuO are 300 nm and 20 nm, respectively. To achieve ideal performance, the doping concentration of CuO should be more than $10^{19}$ cm$^{-3}$, and its hole mobility should be over 1 cm$^2$V$^{-1}$s$^{-1}$. The defect densities in the Sb$_2$Se$_3$ layer and at the CdS/Sb$_2$Se$_3$ interface play a critical role on device performance, both of which should be as low as $10^{13}$ cm$^{-3}$ and $10^{14}$ cm$^{-2}$, respectively. In addition, the work function of the metal electrode should be more than 4.8 eV to avoid formation of Schottky junction at the metal electrode interface. After optimization, a best efficiency of 23.18% can be achieved. Our simulation results provide valuable information to further improve the efficiency of Sb$_2$Se$_3$ solar cells in practice.

1. Introduction
Antimony selenide (Sb$_2$Se$_3$) is a p-type semiconductor material [1] with an orthogonal crystal structure. It has a high absorption coefficient ($>10^5$ cm$^{-1}$) [2], a direct band gap of 1.1–1.3 eV [3], and a good hole mobility up to $2 \times 10^{-2}$ cm$^2$V$^{-1}$s$^{-1}$ [4]. Moreover, both Sb and Se are comparatively earth-abundant, low-cost, and low-toxic. These will make Sb$_2$Se$_3$ a promising material for photovoltaics in the future.

In 2009, Sb$_2$Se$_3$ film began to be used as an absorber layer for solar cells, which was prepared by Messina et al using chemical bath deposition (CBD) with a conversion efficiency of only 0.66% [5]. In 2014, Zhou et al prepared Sb$_2$Se$_3$ thin film by spin-coating and low-temperature sintering, and they made the FTO/TiO$_2$/Sb$_2$Se$_3$/Au heterojunction solar cell with an efficiency of 2.26% [6]. In the same year, Luo et al fabricated superstrate CdS/Sb$_2$Se$_3$ solar cells by thermal evaporation with an efficiency of 1.9% [7]. Subsequently, Leng et al introduced an additional selenization step into the thermal evaporation process of Sb$_2$Se$_3$, which reduced the deep defect density of selenium vacancy, caused by Se loss in Sb$_2$Se$_3$ thin films during normal evaporation, and the device efficiency was further improved to 3.7% [8]. In 2015, Zhou et al grown high-quality Sb$_2$Se$_3$ film with one dimensional crystal structure by using rapid thermal evaporation (RTE), and the device achieved an efficiency of 5.6% [9]. In 2017, Chen et al introduced PbS colloidal quantum dot film as a hole transport layer (HTL) to alleviate carrier recombination loss, and the efficiency was increased to 6.5% [10]. In 2018, Wen et al used the vapor transport deposition (VTD) method to deposit Sb$_2$Se$_3$ film along the [221] orientation to enhance carrier transport, and the efficiency was increased to 7.6% [11]. In 2019, Li et al used the close-packed sublimation (CSS) technique to successfully grow Sb$_2$Se$_3$ nanorod arrays along the [001] orientation on the Mo electrode, and the highest efficiency of 9.2% to date was achieved [12].

Despite such rapid progress, the open-circuit voltage ($V_{OC}$) and short-circuit current density ($J_{SC}$) of Sb$_2$Se$_3$ solar cells are far from being ideal. To further improve device performance, quite a few parameters need to be investigated, resulting in a tremendous burden for experimental research. Therefore, theoretical simulations...
offer us a quick and effective way to study these key parameters, which might provide valuable ideas for experimental work.

In this work, we used SCAPS software to simulate the performance of FTO/CdS/Sb2Se3/HTL/Au superstrate configuration solar cells with different HTLs including CuSCN, CuI, PEDOT:PSS and CuO. The parameters such as thickness, doping concentration, hole mobility, defect density, and metal work function have been systematically studied.

2. Simulation model

2.1. Device structure

The device structure in our simulation is glass substrate/FTO/CdS/Sb2Se3/HTL/Au, as shown in figure 1 (a). FTO is applied as a front electrode collecting electrons. CdS is n-type, used as an electron transport layer (ETL). Sb2Se3 is p-type, which is used as an absorption layer. Au is used as a rear electrode collecting holes. The HTL inserted between Sb2Se3 and Au includes CuSCN, CuI, PEDOT:PSS and CuO.

The energy band diagram of the device using different materials as HTL is shown in figure 1 (b). The conduction band offset (CBO) at the CdS/Sb2Se3 interface is 0.15 eV, which can promote the movement of photoelectrons to the forward electrode. There is also a valence band offset (VBO) at the Sb2Se3/HTL interface, which will affect holes to transport to Au electrode. Moreover, there is a conduction band barrier at the Sb2Se3/HTL interface, and electrons can be reflected from this interface, leading to a less recombination rate to improve device performance.

2.2. Numerical equations

SCAPS is an effective tool to simulate the performance of solar cells, which is developed by University of Gent, and can provide good agreement between experiment and simulation results [13]. Therefore, the SCAPS is used to simulate the Sb2Se3 solar cell. The theoretical calculation is mainly based on three basic equations, which are the Possion’s equation, carrier continuity equation, and the drift-diffusion equation:

\[ \frac{\partial^2 \varphi}{\partial x^2} = \frac{q}{\varepsilon} (n - p) \]  
\[ \frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + G - R \quad \frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} + G - R \]  
\[ J_n = q D_n \frac{\partial n}{\partial x} - q \mu_n n \frac{\partial \varphi}{\partial x} \quad J_p = -q D_p \frac{\partial p}{\partial x} - q \mu_p p \frac{\partial \varphi}{\partial x} \]

Where \( \varphi \) is electric potential, \( q \) is electron charge, \( \varepsilon \) is dielectric constant, \( n \) is electron concentration, \( p \) is hole concentration, \( J_n \) is electron current density, \( J_p \) is hole current density, \( G \) is carrier generation rate, and \( R \) is carrier recombination rate. \( D_n \) and \( D_p \) are electron and hole diffusion coefficient, respectively, and \( \mu_n \) and \( \mu_p \) are electron and hole mobility, respectively.

The absorbing layer defect is set to neutral Gaussian distribution with a characteristic energy of 0.1 eV, and the defect density (\( N_t \)) of Sb2Se3 layer is initially set as \( 10^{14} \) cm\(^{-3} \). The interface defect density plays a key role on device performance, so initial choice of the \( N_t \) values should be careful. In our simulation, the \( N_t \) is initially set as \( 10^{17} \) cm\(^{-2} \) and \( 10^{16} \) cm\(^{-2} \) at the CdS/Sb2Se3 and Sb2Se3/HTL interfaces, respectively. The absorption coefficient and refractive index of Sb2Se3 are from reference [14]. The hole and electron surface recombination
The rate are both set as $10^7 \text{cm s}^{-1}$. The operating temperature is 300 K and the illumination spectrum is global AM 1.5. The material parameters of the device simulation are chosen from the literature [15–22], and summarized in table 1.

### Table 1. Simulation parameters of Sb$_2$Se$_3$ solar cells.

| Material properties | CuO | CuI | PEDOT: PSS | CuSCN | Sb$_2$Se$_3$ | CdS |
|---------------------|-----|-----|------------|-------|-------------|-----|
| Thickness (nm)       | 30  | 30  | 30         | 30    | 600         | 50  |
| Bandgap (eV)         | 2.1 | 2.98| 2.2        | 3.4   | 1.2         | 2.4 |
| Electron affinity (eV)| 3.2 | 2.1 | 2.9        | 1.9   | 4.04        | 4.2 |
| Relative dielectric permittivity | 7.11 | 6.5 | 3.0   | 10    | 18          | 10  |
| CB effective density of states (cm$^{-3}$) | $2.2 \times 10^{20}$ | $2.8 \times 10^{19}$ | $2.2 \times 10^{15}$ | $1.7 \times 10^{19}$ | $2.2 \times 10^{18}$ | $2.2 \times 10^{18}$ |
| VB effective density of states (cm$^{-3}$) | $5.5 \times 10^{19}$ | $1.0 \times 10^{19}$ | $1.8 \times 10^{19}$ | $2.5 \times 10^{19}$ | $1.8 \times 10^{19}$ | $1.8 \times 10^{19}$ |
| Electron mobility (cm$^2$ V$^{-1}$ s$^{-1}$) | 3.4 | $1.7 \times 10^{-4}$ | $2.0 \times 10^{-2}$ | $1.0 \times 10^{-4}$ | 15 | 100 |
| Hole mobility (cm$^2$ V$^{-1}$ s$^{-1}$)   | 3.4 | $1.7 \times 10^{-4}$ | $2.0 \times 10^{-4}$ | $1.0 \times 10^{-4}$ | 5.1 | 25 |
| Acceptor doping N$_A$ (cm$^{-3}$) | $10^{18}$ | $10^{18}$ | $10^{18}$ | $10^{18}$ | $10^{13}$ | $10^{18}$ |
| Donor doping N$_D$ (cm$^{-3}$) | 0 | 0 | 0 | 0 | 0 | $10^{18}$ |

### Table 2. $V_{OC}$, $J_{SC}$, FF and PCE of Sb$_2$Se$_3$ solar cells with different HTLs.

| Parameter | $V_{OC}$ (V) | $J_{SC}$ (mA cm$^{-2}$) | FF (%) | PCE (%) |
|-----------|--------------|------------------------|--------|---------|
| Without   | 0.504        | 32.58                  | 63.10  | 10.37   |
| CuSCN     | 0.648        | 33.55                  | 66.29  | 14.40   |
| CuI       | 0.635        | 33.16                  | 63.38  | 13.34   |
| CuO       | 0.650        | 33.93                  | 66.75  | 14.70   |
| PEDOT: PSS| 0.648        | 33.25                  | 59.97  | 12.92   |

Figure 2. Sb$_2$Se$_3$ solar cell with different HTLs (a) J-V curve, (b) Energy level alignment diagram.

3. Results and discussion

3.1. Device performance with different HTLs

The J-V curves of the devices with different HTLs are shown in figure 2(a), and the device performance parameters are summarized in table 2. When there is no HTL, the $V_{OC}$ is 0.504 V and the power conversion efficiency (PCE) is 10.37%. With the addition of HTL, the $V_{OC}$ and PCE have been significantly improved. As shown in figure 2(b), the presence of conduction band barrier at the Sb$_2$Se$_3$/HTL interface can reflect electrons away, resulting in a less recombination rate to enhance device performance. As indicated in table 2, the device with CuO as a HTL has the best performance, where $V_{OC}$ is 0.650 eV, $J_{SC}$ is 33.93 mA cm$^{-2}$, fill factor (FF) is 66.75%, and PCE is 14.70%. Therefore, we choose CuO as the HTL material to further discuss the effects of other parameters on device performance.
3.2. Influence of Sb$_2$Se$_3$ absorption layer thickness

The thickness of Sb$_2$Se$_3$ layer plays an important role in solar cells. We have investigated the effect of absorber layer thickness on device performance in the range of 100–1200 nm. As shown in figure 3(a), the $V_{OC}$ reaches the optimal value of 0.649 V at 600 nm, and then decreases slightly when the absorber layer thickness is further increased, which should be due to the fact that the recombination rate can be enhanced in a thick film.

As shown in figure 3(b), $J_{SC}$ increases significantly when the absorption layer thickness is up from 100 to 500 nm, and then it decreases gradually after 500 nm. The maximum $J_{SC}$ value of 34.06 mA cm$^{-2}$, at a thickness of 500 nm, is mainly due to saturation absorption of the Sb$_2$Se$_3$ layer. As the thickness of the absorption layer is further increased, which is larger than the diffusion length, the carrier recombination enhancement in a thicker layer leads to the decrease of $J_{SC}$.

Figure 3(c) shows that FF decreases monotonically from 79.1% to 58.8% as the thickness of the absorption layer is changed from 100 to 1200 nm. FF represents the characteristic of maximum power output when the solar cell is connected to the optimal load. The internal resistance is increased when the absorption layer thickness becomes thicker, and the depletion is enhanced, leading to the decrease of fill factor [23].

As shown in figure 3(d), the PCE increases and reaches a maximum value of 16.11% at 300 nm, and then decreases with further increase of Sb$_2$Se$_3$ layer thickness. In the simulation, the cell efficiency is mainly determined by two factors: light absorption and carrier transportation. When the absorption layer is thin (e.g. <300 nm), light absorption becomes a dominant factor determining the efficiency of the cell. Because, the thickness of the absorption layer is less than the carrier diffusion length, so that most carriers can reach the corresponding electrode and the efficay is not limited by carrier transport. When the absorption layer is thick, carrier transport is a dominant factor determining the efficiency of the cell because the light absorption is saturated when the absorption thickness is over the critical value. Based on interaction between these two factors, the Sb$_2$Se$_3$ solar cell at a thickness of 300 nm has the best performance, where the PCE is 16.06%, $V_{OC}$ is 0.643 V, $J_{SC}$ is 33.54 mA cm$^{-2}$, and FF is 74.43%.

3.3. Influence of CuO thickness

In this section, we will discuss the effect of CuO thickness on device performance. The main function of CuO as a HTL is to transport photogenerated holes to the metal electrode. As shown in figure 4, $V_{OC}$ is increased when the thickness of CuO layer is from 1 to 15 nm, and then keeps nearly constant after 15 nm. By comparison, the enhancement of $J_{SC}$ is slight, indicating that the thickness of HTL is almost independent of $J_{SC}$. Similar to $V_{OC}$.
FF is enhanced when the CuO thickness is from 1 to 20 nm, and then keeps almost constant after 20 nm. Thus, the PCE is continuously increased when the CuO thickness is raised from 1 to 20 nm, and tends to keep constant after 20 nm, reaching a highest value of 16.06%. Therefore, the CuO thickness is set as 20 nm for further simulation.

### 3.4. Influence of the doping concentration of CuO layer

The doping concentration ($N_A$) of CuO is an important factor affecting device performance. As shown in Figure 5(a), when $N_A$ is raised from $10^{16}$ to $10^{19}$ cm$^{-3}$, $V_{OC}$ is significantly increased from 0.556 to 0.643 V, and begins to saturate after $10^{18}$ cm$^{-3}$. But $J_{SC}$ is slightly enhanced from 32.58 to 33.61 mA cm$^{-2}$ with the same rise of $N_A$, and the PCE is increased from 11.48% to 16.15% correspondingly. Figure 5(b) shows energy band diagram of the Sb$_2$Se$_3$ solar cell with different doping concentrations of CuO layer. When the $N_A$ of CuO is increased, the valence band of CuO layer will be closer to the quasi-fermi energy level, leading to enhancement of the internal electric potential at the Sb$_2$Se$_3$/CuO interface. Therefore, a higher $V_{OC}$ can be achieved. Figure 5(c) shows the external quantum efficiency diagram. The external quantum efficiency increases slightly with the raise of $N_A$, resulting in a limited improvement of $J_{SC}$, which is in agreement with $J_{SC}$ variation in the J-V curve of figure 5(a).

Both the hole mobility ($\mu_p$) and $N_A$ of CuO layer can affect device performance, as shown in figure 5(d). When the $N_A$ is $10^{15}$ cm$^{-3}$ and $\mu_p$ is $10^{-3}$ cm$^2$ V$^{-1}$ s$^{-1}$, the device efficiency is only 8.97%, which is mainly due to the low conductivity of CuO layer. As $N_A$ and $\mu_p$ increase, so does the PCE. When $\mu_p$ is increased from 1 to 100 cm$^2$ V$^{-1}$ s$^{-1}$, its impact on device efficiency is negligible. Compared to $\mu_p$, $N_A$ is much more sensitive on device performance. When $\mu_p$ is set as 1 cm$^2$ V$^{-1}$ s$^{-1}$ and $N_A$ is increased from $10^{13}$ to $10^{19}$ cm$^{-3}$, the efficiency is raised from 11.29% to 16.15%.

### 3.5. Influence of the defect density of the absorption layer

The impact of the defect density in the Sb$_2$Se$_3$ layer on device performance is of great importance [24]. Since the photogenerated current is mainly produced by the Sb$_2$Se$_3$ layer, the high defect density leads to an increase in carrier recombination, affecting device efficiency. In this study, the effect of the defect density in the range of $10^{13}$ to $10^{18}$ cm$^{-3}$ on device performance has been investigated. Figure 6(a) shows the J-V characteristics of the Sb$_2$Se$_3$ solar cell with different defect densities in the absorber layer. It can be noted that increasing the defect density from $10^{13}$ to $10^{18}$ cm$^{-3}$ leads to a significant decline in device performance. When Sb$_2$Se$_3$ layer defect density is less than $10^{14}$ cm$^{-3}$, the device performance remains almost unchanged, and the optimal PCE can reach 16.25%. As shown in figure 6(b), the recombination rate in the Sb$_2$Se$_3$ layer can seriously affected by the defect density. The increase of defect density leads to a rise of carrier recombination rate. Accordingly, carrier lifetime and diffusion length decrease, and the device performance declines. When the defect density of the
The absorption layer is $10^{18}$ cm$^{-3}$, the carrier generation rate is close to the recombination rate, which results in the device efficiency of only 0.41%. Therefore, in order to improve the performance of Sb$_2$Se$_3$ devices in the experiment, we should try to lower the Sb$_2$Se$_3$ defect density as low as possible. According to the literature [9, 12], by controlling [Sb$_4$Se$_6$]$_n$ atomic chains, the Sb$_2$Se$_3$ film can grow along the [001] direction perpendicular to the p-n junction interface, which can lower the defect density, leading to a high efficiency.

### 3.6. Influence of interface defect density

It has been reported that the carrier recombination that occurs at the CdS/Sb$_2$Se$_3$ interface in the device can affect the $V_{OC}$ [25]. Since the light is incident from the front electrode, the amount of photogenerated carriers at
the CdS/Sb$_2$Se$_3$ interface are much more than at the Sb$_2$Se$_3$/CuO interface. It is well known that the recombination rate depends on the amount of excess carrier density. So the investigation of the defect density ($N_t$) at the CdS/Sb$_2$Se$_3$ interface is more important.

Figure 7 shows the J-V characteristics of Sb$_2$Se$_3$ solar cell with different defect densities at the CdS/Sb$_2$Se$_3$ interface when the defect density of the absorption layer is set as $10^{13}$ cm$^{-3}$. The device performance continues to decrease with the increase of interface $N_t$ in the range of $10^{14}$ to $10^{18}$ cm$^{-2}$ because carrier recombination can be enhanced when the interface $N_t$ increases, resulting in a decrease in PCE. The best PCE can reach 23.18% when the interface $N_t$ is $10^{14}$ cm$^{-2}$.

3.7. Influence of metal work function

In this section, the effect of different metal work functions on device performance has been investigated. As shown in figure 8, when CuO is as used as the HTL, the efficiency decreases as the work function of the metal electrode declines from 4.8 to 4.4 eV, and there is a negligible improvement on device performance when the work function is increased from 4.9 to 5.1 eV. When the work function is less than 4.8 eV, there will be an obvious energy-level mismatch at the CuO/metal interface, resulting in the formation of a Schottky junction, and the device efficiency is negatively affected. When the work function is over 4.8 eV, the device efficiency can reach the optimal value of 23.18%. Therefore, in order to realize the high efficiency of Sb$_2$Se$_3$ solar cells, it is important to choose an appropriate metal electrode. Our investigation suggests that the metal with the work function higher than 4.8 eV should be suitable for the back electrode of Sb$_2$Se$_3$ solar cells.
4. Conclusion

In summary, SCAPS software was used to simulate the performance of the Sb$_2$Se$_3$ solar cells with a configuration of FTO/Cds/Sb$_2$Se$_3$/HTL/Au. The simulation results show that insertion of an appropriate HTL between Sb$_2$Se$_3$ and Au electrode can enhance device performance and CuO is the best choice with the PCE increasing from 10.37% to 14.70%. Several parameters are carefully investigated after the choice of CuO as a HTL. The optimum thicknesses of Sb$_2$Se$_3$ and CuO are 300 nm and 20 nm, respectively. For better performance of the device, the hole mobility of CuO should be over 1 cm$^2$ V$^{-1}$ s$^{-1}$ and its doping concentration should be greater than 10$^{19}$ cm$^{-3}$. To reach a best efficiency of 23.18%, the defect densities in the Sb$_2$Se$_3$ layer and at the CdS/Sb$_2$Se$_3$ interface should be as low as 10$^{13}$ cm$^{-3}$ and 10$^{14}$ cm$^{-2}$, respectively, both of which play a critical role on device performance. Finally, to avoid forming Schottky junction at the CuO/metal electrode interface, the metal electrode with the work function more than 4.8 eV should be used.

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