



Simulation the Effect of Back Reflector Layer Addition, Doping, and Thickness on Solar Cell Performance

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ABSTRACT

The solar cell structure "glass/Mo(Molybdenum)/Sb₂S₃(Antimony sulfide)/CdS (Cadmium sulfide)/i:ZnO (Zinc oxide)/Al:ZnO" (Aluminium-doped Zinc Oxide) was simulated using the solar cell capacitance simulator (SCAPS), and the results showed good agreement with the original Sb₂S₃ cell performance. Adding multiple layers of back reflection increased cell efficiency. Among these, the CuSb₂S₃ (Antimony-copper sulfide) layer yielded the best performance, raising the efficiency from (11.43 %) to (20.59 %). Further improvement was achieved by increasing the impurity concentration in the best back-reflection layer, which improved efficiency from (20.59 %) to (23.16 %). Additionally, increasing the absorber-layer thickness further increased efficiency to (26.22 %) with a fill factor of (89.36 %).

Keywords: *Acceptor Doping, SCAPS, Simulation, Solar Cell.*

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محاكاة تأثير إضافة طبقة انعكاس خلفي والتشويب والسلك على الخلية الشمسية

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الملخص

تمت محاكاة بنية الخلية الشمسية ذات التركيب Mo/(المولبيدينوم)Sb₂S₃/(كبريتيد الانتيمون)CdS/(كبريتيد الكاديوم)i:ZnO/(أكسيد الزنك)Al:ZnO/(أكسيد الزنك المطعم بالألمنيوم) باستخدام برنامج SCAPS-1D، حيث أظهرت نتائج المحاكاة توافقاً جيداً مع مؤشرات الأداء الخاصة بالخلية المرجعية التجريبية. بعد ذلك، تم إدخال طبقات انعكاس خلفي مختلفة، مما أدى إلى تحسن كبير في كفاءة الجهاز. من بين هذه الطبقات، أظهرت طبقة (كبريتيد الانتيمون والنحاس) CuSb₂S₃ أفضل أداء، حيث ارتفعت الكفاءة من (11.43 %) إلى (20.59 %)، وتم تحقيق تحسين إضافي من خلال زيادة تركيز الشوائب في أفضل طبقة انعكاس خلفي، مما أدى إلى رفع الكفاءة إلى (23.16 %). بالإضافة إلى ذلك، ساهمت زيادة سمك طبقة الامتصاص في تحقيق كفاءة قصوى بلغت (26.22 %) مع عامل الملى بلغ (89.36 %).

1. INTRODUCTION

Nowadays, most global energy comes from fossil fuels. The world consumed 13,647 Mtoe (Million Tonnes of Oil Equivalent) of energy in 2015, with nuclear and fossil fuels accounting for more than (86 %) of this total. However, fossil fuels are scarce and cause pollution by releasing harmful pollutants such as carbon dioxide and heavy metals like arsenic, which are extremely harmful to human health ⁽¹⁾. Photovoltaic (PV) systems, now recognized as renewable, clean, and sustainable, have attracted considerable interest because they can directly convert sunlight into electrical energy. Second, their theoretical efficiency is relatively higher than that of other energy sources. Third, PV technology has no moving parts, which prevents wear and tear from mechanical movement. PV systems can operate continuously with minimal maintenance, and semiconductors are essential materials for PV energy ⁽²⁾. Semiconductors absorb photons with energies higher than their bandgap and then radiate, heat, or otherwise release the excess energy. Much work has focused on increasing efficiency by developing different types of solar

cells ⁽³⁾. Antimony sulfide (Sb₂S₃) is a promising material for solar cell fabrication due to its favorable optoelectronic properties. It exhibits high stability, a direct bandgap of 1.6 eV, and an absorption coefficient of about $1 \times 10^5 \text{ cm}^{-1}$. Moreover, it is abundant and environmentally friendly ⁽⁴⁻⁶⁾. Sb₂S₃ has been widely used in electronic applications, photovoltaic devices, photodetectors, and photoelectrochemical cells ⁽⁷⁾. Numerous studies have confirmed the high absorptivity of Sb₂S₃, making it suitable for use in solar cells and sensitized devices ⁽⁸⁾. Adding a back-reflection layer to the solar cell increases energy absorption by increasing the rate of electron-hole pair generation, thereby improving cell performance ⁽⁹⁾. In this study, we used Sb₂S₃ as the absorber layer. We first simulated the original Sb₂S₃ solar cell structure, then introduced various back reflector layers. We then further optimized the best-performing cell by increasing the back-reflector doping concentration and the absorber-layer thickness.

2. MODELING

2.1 Numerical Simulation Using SCAPS

The Department of Electronics and Information Systems (ELIS) at the University of Gent, Belgium, created the one-dimensional solar cell simulation tool SCAPS (Solar Cell Capacitance Simulator) ^(10, 11). SCAPS operates by numerically solving semiconductor equations, beginning with the Poisson equation ⁽¹²⁾.

$$\nabla(E) = \frac{q}{\epsilon} (p - n + N_D^+ - N_A^-) \quad (1)$$

Where (E) is the electric field, (q) is the elementary charge, (ϵ) is the permittivity of the absorber, (n and p) represent the density of electrons and holes, respectively, and (ND and NA) are the donor and acceptor concentrations, respectively. The continuity equation follows from the following relation. ⁽¹³⁾:

$$\frac{dn}{dt} = \frac{1}{q} (\nabla(J_n) + G_n - R_n) \quad (2)$$

$$\frac{dp}{dt} = -\frac{1}{q} (\nabla(J_p) + G_p - R_p) \quad (3)$$

where (J_n and J_p) are the electron and hole current densities, respectively; (G_n and G_p) are the electron and hole generation rates, respectively; and (R_n and R_p) are the electron and hole recombination rates. Lastly, the following equations provide the charge-carrier formulae for drift and diffusion current densities. ⁽¹⁴⁾.

$$J_n = q(\mu_n n E + D_n \nabla n) \quad (4)$$

$$J_p = q(\mu_p p E + D_p \nabla p) \quad (5)$$

Where (μ_n and μ_p) are the electron and hole mobilities, respectively, and (D) is the diffusion constant. Finding the fill factor (FF), open-circuit voltage (Voc), short-circuit current density (Jsc), and conversion efficiency (η) is crucial for assessing the performance of solar cells since these variables are connected by the following equations ⁽¹⁴⁾.

$$FF = \frac{P_{max}}{P_t} = \frac{V_{max} \cdot J_{max}}{V_{oc} \cdot J_{sc}} \quad (6)$$

$$\eta = \frac{P_m}{P_{in}} = \frac{V_{oc} \cdot J_{sc} \cdot FF}{P_{in}} \quad (7)$$

Where (V_{max}) is the maximum voltage, (P_{max}) is the maximum power, (I_{max}) is the maximum current, and (P_{in}) is the Incoming power. A relationship exists between current and potential difference.

$$V_{oc} = \frac{KT}{q} \ln \left(\frac{I_L}{I_0} - 1 \right) \approx \frac{KT}{q} \ln \left(\frac{I_L}{I_0} \right) \quad (8)$$

Where (K) is Boltzmann's Constant, (T) is temperature in Kelvin, (I_0) represents the Saturation current of the diode, and its equation is:

$$I_0 = DT^3 \exp \left[\frac{-E_g}{KT} \right] = A \left[\frac{q D_e n_i^2}{L_e N_A} + \frac{q D_h n_i^2}{L_h N_D} \right] \quad (9)$$

Where (E_g) is the energy gap, (L_e and L_h) are the diffusion lengths of electrons and holes, respectively, and (A) is the diode cross-section. It is possible to calculate the minority carrier lifetime, which correlates with the recombination rate and doping concentration and indicates the average time a minority carrier remains before recombining. The following relation provides it. ⁽¹⁵⁾:

$$\tau = \frac{1}{\sigma V_{th} N_t} \quad (10)$$

$$\tau = \frac{\Delta n}{U} \quad (11)$$

Where (τ) is the minority carrier lifetime, (N_t) is the defect concentration, (V_{th}) is the thermal speed, (σ) is the conductivity, (U) is the recombination rate, and (Δn) is the excess minority carrier concentration.

2.2 Cell Structure

The experimental solar cell structure generally consists of a glass substrate with deposited molybdenum, followed by the absorber layer, antimony sulfide (Sb_2S_3). This material has a relatively small bandgap, enabling efficient light absorption. On top of the absorber, a cadmium sulfide (CdS) buffer layer is deposited; its moderate bandgap allows a significant portion of light to pass through to the absorber layer. Next, a zinc oxide (ZnO) bilayer is added, comprising an intrinsic (i:ZnO) layer followed by an aluminum-doped ZnO (Al: ZnO) layer. This bilayer has a high bandgap (~3.3 eV) and acts as a transparent window that facilitates light transmission into the underlying absorber layer. The complete cell configuration follows the order: glass/Mo/ Sb_2S_3 /CdS/i: ZnO/Al: ZnO. The device features a front contact operating under flat-band conditions, a rear contact composed of molybdenum (Mo) interfacing with the absorber layer, and an aluminum contact with a work function of approximately 5 eV. The cell is

constructed on a glass substrate ⁽¹⁶⁾. Table (1) presents the simulation parameter values used in the modeling process, all set at a standard operating temperature of 300 K. Figure (1) illustrates the detailed structure of the solar cell.

Table 1: The physical parameters of different layers ⁽¹⁷⁻¹⁹⁾.

Parameters	Symbol	Sb ₂ S ₃	CdS	i-ZnO	AZO
Thickness	W (μm)	1	0.05	0.05	0.3
Bandgap	E _g (eV)	1.6	2.4	3.3	3.3
Electron affinity	χ (eV)	3.7	4.2	4.55	4.55
Dielectric permittivity	ε _r	7.08	9	8	8
CB effective density of states	N _C (cm ⁻³)	2.63×10 ¹⁹	1×10 ¹⁸	1×10 ¹⁸	1×10 ¹⁸
VB effective density of states	N _V (cm ⁻³)	2.25×10 ¹⁹	1×10 ¹⁹	8×10 ¹⁸	1×10 ¹⁸
Electron thermal velocity	V _n (cm/s)	1×10 ⁷	1×10 ⁷	1×10 ⁷	1×10 ⁷
Hole thermal velocity	V _p (cm/s)	1×10 ⁷	1×10 ⁷	1×10 ⁷	1×10 ⁷
Electron mobility	μ _n (cm ² /v.s)	50	50	100	100
Hole mobility	μ _p (cm ² /v.s)	10	20	25	20
Shallow uniform donor density	N _D (1/cm ³)	0	1×10 ⁷	1×10 ¹⁰	1×10 ²⁰
Shallow uniform acceptor density	N _A (1/cm ³)	5e15	0	0	0
Coefficient absorption	α (1/cm)	5.0×10 ⁴	scaps	scaps	scaps

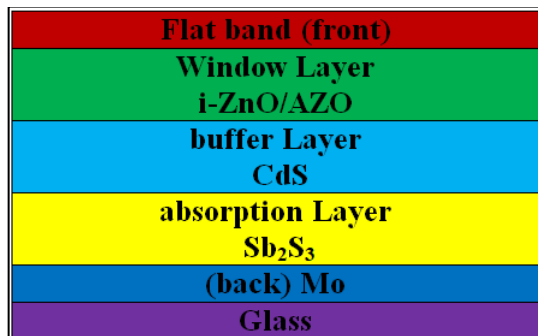


Fig. 1: Experimental cell structure.

3. RESULTS AND DISCUSSION

After simulating the solar cell with the structure glass/Mo/Sb₂S₃/CdS/i-ZnO/Al: ZnO, the results were consistent with those of the experimental cell. Table (2) compares the outputs of the simulated and real cells. Figure (2) shows the cell's energy band levels, illustrating the potential barrier between the

absorption layer and the buffer layer, as well as between the buffer layer and the window layer. This increases cell efficiency by returning electrons to the other end and preventing accumulation, thereby reducing recombination. ⁽¹⁵⁾.

Table 2: Comparison of Solar Cell Outputs Between the Experimental and Simulated Structures

No.	Cell Type	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	η (%)
1	Experimental Sb ₂ S ₃ Cell	0.967	19.18	61.82	11.47
2	Simulated Cell	0.996	18.74	61.20	11.43

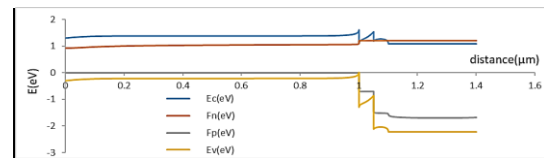


Fig. 2: Experimental solar cell energy levels.

3.1 Effect of Back Reflector Layers

We added different back reflector layers beneath the absorber layer (Sb₂S₃), using materials such as SnS, Si, CIGS, CZTSSe, and CuSbS₃. Table (3) presents the output parameters of the cell before and after the addition of these back reflector layers. Figure (3) shows a noticeable effect on the current-voltage (I–V) characteristics. This improvement is attributed to the absorber layer receiving more incident light reflected by the back reflector layer. Table (4) lists the material parameters of the layers used as back reflectors in the cell. The rear reflector layer improves both conversion efficiency and fill factor by reflecting incident electrons that pass through the absorber layer. This reduces recombination, increases charge-carrier concentration, improves ohmic contact, and yields a higher photocurrent ⁽²⁰⁾. From these findings, it can be concluded that the most effective back reflector layer was CuSbS₃, which increased the conversion efficiency from (11.43 %) in the experimental cell to (20.59 %) in the modified cell. This improvement can be attributed to two main factors ^(21, 22):

1. Because of the higher potential barrier caused by the reflector layer's low electron affinity, more electrons are reflected from the rear surface.
2. The sum of the electron affinity and the energy bandgap of the back reflector layer is equal to or slightly higher than the work function, which enhances ohmic conductivity when their values are closely matched.

Table 3: The output parameters of the experimental cell compared to the cell with various back reflector layers

Material	Jsc (mA/cm ²)	Voc (V)	Fill Factor (%)	Efficiency (%)
Experimental Cell	18.74	0.996	61.2	11.43
(SnS)	20.60	1.01	66.68	13.94
(Si)	16.00	1.11	80.77	14.37
(CIGS)	16.92	1.11	81.41	15.39
(CZTSSe)	19.50	1.13	83.68	18.53
(CuSbS ₃)	22.11	1.06	87.53	20.59

Table 4: The parameters of the back reflector layers used (23-27).

Parameters	symbol (unit)	SnS	Si	CIGS	CZTSSe	CuSbS ₃
W	(μm)	0.1	0.1	0.05	0.05	0.05
Eg	(eV)	1.1	1.12	1.05	1.3	1.5
X	(ev)	4.2	4.05	4.14	4.1	4.2
Dielectric permittivity	ε _r	12.5	11.9	10	13.6	10
N _c	(cm ⁻³)	1×10 ¹⁹	2.58×10 ¹⁹	1×10 ¹⁸	2.2×10 ¹⁸	2.2×10 ¹⁸
N _v	(cm ⁻³)	4.1×10 ¹⁹	2.65×10 ¹⁹	1×10 ¹⁸	1.8×10 ¹⁹	1.8×10 ¹⁹
V _n	(cm/s)	1×10 ⁷	1×10 ⁷	1×10 ⁷	1×10 ⁷	1×10 ⁷
V _p	(cm/s)	1×10 ⁷	1×10 ⁷	1×10 ⁷	1×10 ⁷	1×10 ⁷
μ _n	(cm ² /v.s)	25	1.35e3	30	100	100
μ _p	(cm ² /v.s)	100	450	15	25	25
N _D	(1/cm ³)	0	0	0	0	0
N _A	(1/cm ³)	1×10 ¹⁸	1×10 ¹⁷	1×10 ¹⁹	1×10 ¹⁹	1×10 ²⁰
α	(1/cm)	5×10 ⁴	5×10 ⁵	5×10 ⁴	5×10 ⁴	5×10 ⁴

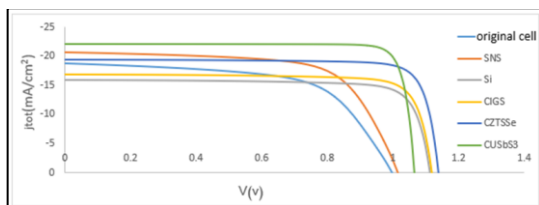


Fig. 3: Solar cell I-V curve before and after adding rear reflector layers.

To understand the impact of the back reflector layer on quantum efficiency (Q.E.), defined as the ratio of collected charge carriers in the solar cell to the

number of incident photons on the cell, refer to Figure 4. This figure shows how quantum efficiency varies with wavelength for different back-reflector arrangements. The variation in Q.E. demonstrates the effect of different back reflector materials. Among them, CuSbS₃ was found to be the most effective, resulting in a power conversion efficiency of (20.59 %). Figure (4) illustrates the quantum efficiency of the solar cell before and after the addition of the back reflector layer larger the energy gap, the shorter the wavelength, and the higher the quantum efficiency. Q.E. increases, peaking around 380 nm. This improvement is attributed to the enhanced absorption of long-wavelength photons reflected by the back reflector layer. As a result, the Q.E. curve becomes more square-like, which represents the ideal case for solar cell operation. (28). Beyond this point, the Q.E. gradually drops to zero around (780 nm), due to reduced carrier diffusion lengths and negligible absorption at longer wavelengths. Therefore, quantum efficiency is inversely related to wavelength, as shown in Equation .

$$Q_E = 1.24 \frac{R_\lambda}{\lambda} \quad (12)$$

where λ is the wavelength, and R_λ is the responsivity from the top surface.

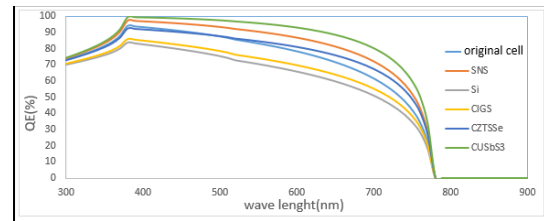


Fig. 4: Quantum efficiency before and after rear reflector layers.

To study the effect of energy level alignment in the solar cell upon the addition of back reflector layers, Figure (2) illustrates the energy band diagram of the original structure (glass/Mo/Sb₂S₃/CdS/i: ZnO/Al: ZnO). The rear interface shows either no potential barrier or a negative potential barrier for electrons, resulting in electron accumulation at the back surface. This accumulation enhances the probability of electron-hole recombination. In contrast, Figure (5) represents the energy band diagram after

incorporating the optimal back reflector layer, forming the modified cell structure (glass/Mo/CuSbS₃/Sb₂S₃/CdS/i: ZnO/Al: ZnO). This configuration creates a high potential barrier for electrons and a low barrier for holes, effectively reflecting many charge carriers toward the absorber layer. As a result, both the open-circuit voltage (V_{oc}) and the short-circuit current density (J_{sc}) increase, leading to an overall enhancement in power conversion efficiency (η)⁽¹⁵⁾.

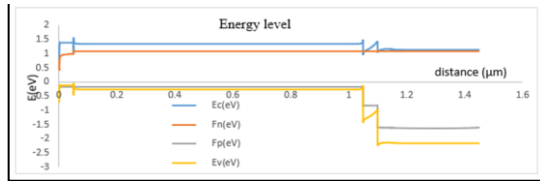


Fig. 5: Energy levels with the ideal rear reflector layer (CuSbS₃) included.

3.2 Effect of Doping the Back Reflector Layer

Figure (6) illustrates the current-voltage (I-V) characteristics for different doping levels. The acceptor doping density in the back reflector layer was varied. The power conversion efficiency increased from (20.23 %) at an acceptor concentration of ($5 \times 10^{19} \text{ cm}^{-3}$) to (23.16 %) at a doping level of ($5 \times 10^{21} \text{ cm}^{-3}$). This improvement is attributed to the fact that increasing N_A enhances the saturation current, which in turn suppresses excess-carrier accumulation and increases the open-circuit voltage (V_{oc})⁽²⁹⁾. Figure (7) shows the effect of doping on quantum efficiency (Q.E.), revealing no significant impact. Figure (8) presents the output parameters of the solar cell under various doping concentrations in the back reflector layer; the cell output increases with increasing doping because increasing doping reduces the reverse saturation current and cell emitters according to equations (6, 7, 8, and 9).

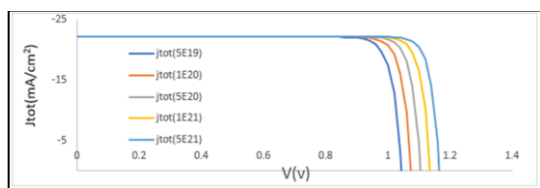


Fig. 6: Voltage as a function of current for different doping levels.

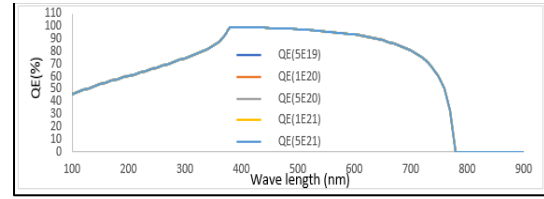


Fig. 7: Quantum efficiency for varying doping levels as a function of wavelength.

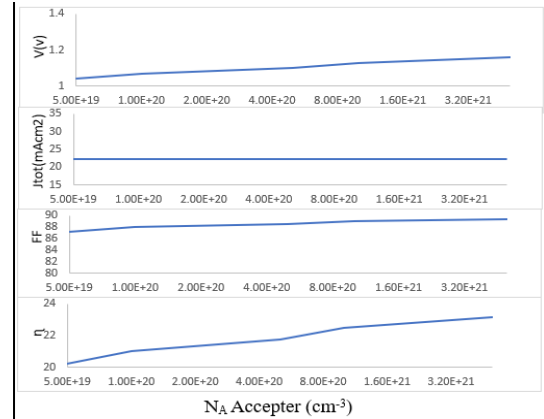


Fig. 8: Solar cell output parameters as a function of doping concentration.

3.3 Effect of Absorber Layer Thickness

Figure (9) illustrates the current-voltage (I-V) relationship for different absorber thicknesses. To investigate the effect of increasing absorber-layer thickness, the thickness was varied from (0.5 μm) to (4 μm). The power conversion efficiency increased from (18.85 %) to (26.22 %). This improvement is attributed to the formation of localized states within the bandgap and the emergence of energy tails as thickness increases, which allow absorption of photons with energies below the bandgap⁽³⁰⁻³²⁾. Figure (10) shows quantum efficiency as a function of wavelength; quantum efficiency increases with thickness because higher absorption rates allow more absorption of low-energy photons, improving cell performance. However, increasing thickness improves performance only to a certain extent, after which it reduces cell efficiency due to increased recombination^(33, 34). Figure (11) represents the results that the short-circuit current and cell efficiency increase with the increase of thickness, while the open-circuit voltage and fill factor remain constant because the increase in thickness increases the generation of electron-hole pairs to some extent, thus increasing the cell efficiency⁽³⁵⁾.

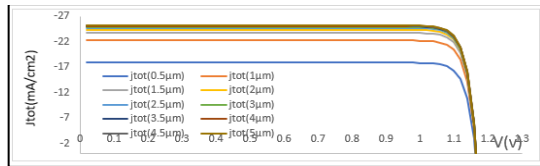


Fig. 9: Voltage as a function of current for different absorber layer thicknesses.

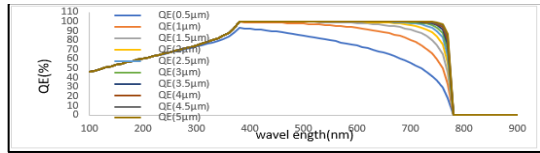


Fig. 10: Quantum efficiency for varying absorber layer thicknesses as a function of wavelength

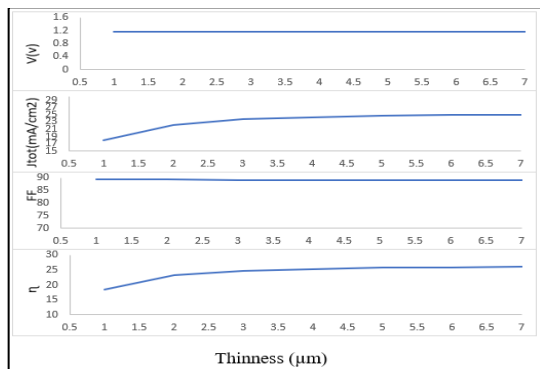


Fig. 11: Solar cell parameters as a function of absorber layer thickness.

4. CONCLUSION

We simulated the solar cell structure (glass/Mo/Sb₂S₃/CdS/i-ZnO/Al: ZnO) using SCAPS-1D, and the results showed good agreement with the experimental cell output. Adding a back-reflector layer improved cell performance by redirecting incident photons that would otherwise pass through the absorber layer. Consequently, recombination decreased, and charge-carrier concentration increased. We also observed improved quantum efficiency, attributed to enhanced absorption of longer-wavelength photons. Additionally, increasing the doping level of the rear reflector layer improved cell efficiency by increasing the saturation current. Increasing the absorber layer thickness increased power conversion efficiency by forming localized states within the bandgap and energy tails that enable absorption of sub-bandgap photons.

Conflicts of Interest: The authors declare that they have no competing interests.

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Author contribution: The authors contributed equally to the study.

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