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Enhancing Photoconversion Efficiency by Optimization of Electron/Hole Transport Interlayers in Antimony Sulfide Solar Cell using SCAPS-1D Simulation

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ABSTRACT

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Absorption layer, Efficiency, Solar Cells, Sb₂S₃, Sb₂Se₃, Photoconversion, optimization, SCAPS-1D. Enhancing photoconversion efficiency in a solar cell with the composition "glass/Mo/ CUSbS₃/ Sb₂S₃/CdS/i:ZnO/AL:ZnO" by varying the thickness of the absorption layer (Sb₂S₃) and adding a secondary absorption layer was performed. The thickness of the original absorption layer (Sb₂S₃) was gradually increased from (1 μ m) to (3.5 μ m). The best efficiency (23.14%) and filling factor (87.52%) were achieved with an absorption layer thickness of 3.5 μ m. This indicates that a thicker absorption layer can enhance efficiency. A secondary absorption layer was introduced between the original absorption layer and the reflection layer.

Several materials were considered for this secondary absorption layer, including MAPbI₃, Sb₂Se₃, CZTS, and CZTSe. The best-performing secondary absorption layer was found to be Sb₂Se₃. The solar cell structure, after combining it with the best reflection layer (CUSbS₃) and the optimized thickness for the original absorption layer (3.5 μ m), was established as "glass/Mo/CUSbS₃/Sb₂Se₃/Sb₂Se₃/CdS/i:ZnO/Al:ZnO".

The optimized solar cell configuration yielded the best conversion efficiency (27.01%) and a high filling factor (85.12%).

These results highlight the significance of layer thickness and the addition of secondary absorption layers in enhancing the solar cell efficiency. The final configuration demonstrates substantial improvements in efficiency and suggests that thoughtful design and material choices can lead to more efficient photovoltaic devices.

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تعزيز كفاءة التحويل الضوئي من خلال تحسين الطبقات البينية لنقل الإلكترون الفجوة في الخلية الشمسية لكبريتيد الأنتيمون باستخدام محاكاة SCAPS-1D .

معتز صالح حسن الجبوري، مبارك حمد عكلم، عبدالقادر على حسن.

ملخص: تتم تحسين كفاءة التحويل الضوئي في الخلية الشمسية ذات التركيب:

(«glass/Mo/CUSbS₃/Sb2S₃/CdS/i:ZnO/AL:ZnO») وذلك بتغيير سمك طبقة الامتصاص (Sb₂S₃) وذلك عند سماكة من («1-3.5 ميكرومتر)، وتم الحصول على أفضل كفاءة (%23.14) وافضل عامل تعبئة (%87.52) وذلك عند سماكة طبقة الامتصاص (3.5) ميكرومتر. يعتبر ذلك مؤشرا إلى أن طبقة الامتصاص الأكثر سمكًا يمكن أن تعزز الكفاءة. بعد ذلك تم إدخال طبقة امتصاص ثانوية بين طبقة الامتصاص الأصلية وطبقة الانعكاس. تم أخذ العديد من المواد في الاعتبار لطبقة الامتصاص الثانوية هذه، بما في ذلك و13.5 وSb₂Se₃ وZTS وSZS وCZTS ، وتم اختيار طبقة الامتصاص (10 Sb₂Se) والسمك الأمثل لطبقة الامتصاص الثانوية هذه، بما في ذلك الخلية الشمسية، بعد دمجها مع أفضل طبقة انعكاس (3.5 من الواد في الأمثل لطبقة الامتصاص الأطلية (3.5 ميكرومتر)، فاصبح تركيبها الجديد هو:

«glass/Mo/CUSbS3/Sb2Se3/Sb2S3/CdS/i:ZnO//Al:ZnO» أسفر التكوين الأمثل للخلايا الشمسية عن أفضل كفاءة تحويل (%27.01) وعامل تعبئة عالي .(%85.12) تسلط هذه النتائج الضوء على أهمية سماكة الطبقة وإضافة طبقات الامتصاص الثانوية في تعزيز كفاءة الخلايا الشمسية. يوضح التكوين النهائي تحسينات كبيرة في الكفاءة ويشير إلى أن التصميم المدروس واختيارات المواد يمكن أن تؤدي إلى أجهزة كهروضوئية أكثر كفاءة.

1. INTRODUCTION

The world's reliance on traditional energy sources is problematic. These sources are finite, and as they deplete, they become more expensive to extract, which can lead to energy shortages. However, fossil fuel consumption not only depletes finite resources but also contributes to environmental pollution and climate change. In addition, the global population grows, energy demand also increases, further straining non-renewable resources. Access to energy is closely linked to urbanization and a higher quality of life. The need to address these challenges has led to a shift toward renewable energy sources. Solar, geothermal energy, hydroelectric power, and wind energy are cleaner, sustainable alternatives to fossil fuels.

Solar energy, in particular, is accessible across most of the Earth's surface. It is renewable, ecofriendly, and locally available. Solar cells, based on the photovoltaic principle, convert sunlight into electricity, providing a reliable and low-maintenance source of power. Solar cells, made from semiconducting materials, play a vital role in capturing and converting solar energy into electrical energy. They offer an environmentally friendly to the world's growing energy needs. Solar cells have gone through different generations and types, with significant advancements in recent years. The photovoltaic industry has played a major role in improving the solar cells efficiency [1].

In 2010, the researcher Soo-Jin Moon [2] and his group studied nanoscale solar cells deposited using a chemical bath method and made from (Sb_2S_3) as a light-absorbing layer deposited on titanium dioxide nanoparticles as organic materials for transporting gaps. The study reported an efficiency of 5.2% for these nanoscales. This efficiency measurement was taken at a solar illuminance of 0.1, indicating that the solar cells were able to convert 5.2% of the incoming light energy into electricity under these conditions.

In 2017, researcher Shi-Joon Sung [3] and his group carried out a systematic control process on the planar solar cells that had of nanostructure interfaces (Sb_2S_3) through a spin coating process and its effect on the photoelectric properties. Research was conducted on the composition and properties of the junction interface between the material. (TiO_2) and (Sb_2S_3) absorption layer for the cell based on (Sb_2S_3) . They found that it is possible for the conditions of interfacial between

the TiO_2 layer and the absorption layer (Sb₂S₃). They proved in this research that the contact between the two layers (TiO₂, Sb₂S₃) affects directly affects the efficiency of solar cell based on antimony sulfide (Sb₂S₃).

Researcher Chharganeh Kalangestani [4] and his group studied in 2020 AD the effect of doping with zinc on the physical properties of thin films with nanostructures of Sb_2S_3 by dipping technique on glass substrates. XRD patterns indicated that the Znx Sb_2S_3 thin films have an orthogonal crystalline structure, and the intensity of the peaks was observed to decrease with increasing zinc doping. Likewise, FESEM images showed that the grain size decreases with increasing zinc concentration. The porosity of the samples also changed with different values of zinc. Also, the optical transmission spectra showed a shift in the absorption edge for different zinc concentrations.

In 2020, researcher Muhammad Ishaq [5] and his group adopted the spray pyrolysis method to precipitate a TiO_2 compound saturated with zinc with levels energy to facilitating the extraction of the charge and transfer. Manufactured of solar cell using the improved TiO_2 ETL is characterized by high interface quality and high voltage construction, thus improving the voltage of open circuit. As a result, the efficiency obtained of 4.41% to 5.16%, which is a record for the open circuit voltage Voc of (702 mV). For free cadmium and inorganic Sb₂S₃.

Numerical simulation and improvement of the solar cell performance (Sb₂S₃) with gap transport layers was conducted by researcher Youpeng Xiao and his group in the year 2020 AD. Simulation of the device's photovoltaic cell performance was conducted using Wx AMPS. The initial values were set for the volumetric density of defect in the Sb₂S₃ layer and the interface density of defect at the interface for both ZnS/ Sb₂S₃ and Sb₂S₃/Cu₂O. The conversion efficiency was increase from 6.24% to 16.65% by incorporating the Cu₂O layer inside cell. The effect of the quality of the bulk Sb₂S₃ materials on the performance of the photovoltaic cell of the device was also analyzed. Conversion efficiency improved of 21.99%, it obtained at an improved Sb₂S₃ thickness layer that could reach 0.8 micrometers. The effect of interface defects for Sb₂S₃/ Cu₂O, ZnS/ Sb₂S₃ was also analyzed. on the photovoltaic of the cell performance [6].

A thin film doped with Sb_2S_3 was prepared by researcher Guochen Ma [7] and his group in the year (2020) AD in order to improve the performance of the organic and inorganic hybrid solar cell. Organic and inorganic hybrid solar cell based on saturated antimony sulfide (Ti) were prepared: Sb_2S_3 using a spin casting method. Compared to cells containing original (Sb_2S_3), the energy conversion efficiency of cells based on Ti: Sb_2S_3 was increased in limits 41%. The effect of the concentration of different Ti impurities on the performance of cells examined. The efficiency of the cells was improved by increasing the concentration of Ti doping until its concentration exceeded 6%, where the highest efficiency rate reached 2.7%. The better performance based on Ti: Sb_2S_3 is due to their improved optical absorption.

Researchers Zhaowen Chen and Guodong Chen (2020) [8] studied the thickness effect of the absorption layer on the solar cell made of planar Sb_2S_3 thin films, where the thickness effect of the solar cell absorber was carefully examined in the range of 80nm - 620nm, With the aim of discovering the difference between charge separation and light absorption inside the cell. Characterization of thin films found that Sb_2S_3 with very thin thickness did not give good efficiency, while Sb_2S_3 that was too thick would hinder charge separation. Finally, the best energy conversion efficiency is 4.96% was accomplish using an absorption thickness of 544 nm.

In 2021, researcher Junweichen [9] and his group used polymer/graphene composite flakes as a gap transport layer in solar cells $(Sb_2S_3)/TiO_2 - BnpHJ$ for the first time. The Sb_2S_3 \TiO₂ - BnpHJ cells provided a conversion efficiency is 5.72% and better stability.

Also, in 2021, the researcrer El-Khozondar [10] and his groupe proposed four structures for solar cells with antireflection coatings, including using sol-gel materials and SiNx. These structures

show potential for low-cost and high-efficiency solar cell production.

In 2022, researcher Jiashuai Li [11] and his group processed the CdS/Sb₂S₃ hybrid junction using an insulating layer of tin oxide (SnO) doped with magnesium for high-efficiency solar cells. Here they introduced a layer of perfluorinated tin oxide. The resulting Sb₂S₃ solar cells with Mg-doped SnO achieved a pioneering advance in efficiency by 6.31%, which is 22.8% higher than those without an insulating layer.

In 2023, the researcher El-Khozondar [12] and his team showed off a cool new solar cell design. It has four layers - NiOx in glass on top of perovskite and SnO₂. Light comes in through the glass and goes out through the substrate. They discovered that changing the thickness of the layers affects how much light gets through, bounces back, or gets absorbed.

Also, in 2023, the researcher Mubarak [13] and his group studied the Sb₂S₃ compound was used as the absorber layer in the solar cell. Different BSL layers were examined, and it found the best reflective layer was to be CUSbS₃, the efficiency of the solar cell was found to be 20.59% with a fill factor of 87.53%.

The research goals for improving the efficiency of the "glass/Mo/CUSbS₃/ Sb₂S₃/CdS/i:ZnO/AL:ZnO" solar cell are as follows:

First: Investigate the impact of substituting the buffer layer (Coping Layer), which plays a crucial role in the cell's efficiency and performance. The choice of the buffer layer can significantly influence the interface between absorption layer and other components of the solar cell.

Second: Analyze the effect of thickness varying of the Sb₂S₃ absorption layer with the performance of solar cell. Adjusting the thickness can influence the amount of light absorbed and electronhole pair generation, which in turn affects the cell's efficiency.

Third: Adding a Second Absorption Layer: Introduce a secondary absorption layer to the solar cell structure and assess its impact on the cell's performance. The addition of this layer may enhance the light absorption and electron generation, further improving the overall efficiency. These research goals are essential for understanding how alterations to different layers within the solar cell structure can enhance its performance and energy conversion efficiency. By systematically studying these factors, researchers can identify the optimal configuration for achieving the highest possible solar cell efficiency.

2. STRUCTURE OF THE SOLAR CELL

As shown in Figure 1. The solar cell under investigation is composed of [14]:

Glass Substrate: The solar cell starts with a glass substrate, which is typically a transparent material to allow sunlight to pass through to the layers below.

Mo (Molybdenum) Back Contact: Molybdenum serves as the back contact of the cell. It is an electrical conductor that collects the electrons generated when sunlight is absorbed by the semiconductor layers.

CUSbS₃ Layer (Back Reflection Layer): CUSbS₃ is used as a back reflection layer in your solar cell. This layer is added to reflect light that has penetrated the Sb₂S₃ absorption layer, redirecting it back into the cell for further absorption. It enhances the cell's performance by increasing the amount of light absorbed.

Sb₂S₃ Absorption Layer: The Sb₂S₃ layer serves as the main absorption layer. It's the core of the solar cell where light is absorbed, and electron-hole pairs are generated. Sb₂S₃ is a semiconductor material that has suitable properties for absorbing sunlight and generating electrical current.

CdS (**Cadmium Sulfide**) **Layer:** CdS is a semiconductor layer that is used as a buffer layer. It helps improve the interface between the Sb₂S₃ absorption layer and the next layer, which is the i:ZnO layer. It assists in electron transport and can act as an electron-blocking layer.

i:ZnO (Intrinsic Zinc Oxide) Layer: The intrinsic zinc oxide layer is also known as the window

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layer. It allows light to pass through while helping to transport electrons generated within the cell. **Al:ZnO (Aluminum-Doped Zinc Oxide) Front Contact:** The Al:ZnO layer serves as the front electrical contact of the solar cell. It collects the electrons from the cell and allows them to be extracted for external use.



Figure 1. The schematic Structure Solar Cell.

3. DESCRIPTION PERFORMANCE OF SOLAR CELL

The exact performance characteristics of our solar cell structure (glass/Mo/CuSbS₃/ Sb₂S₃/ CdS/i:ZnO/AL:ZnO), would depend on the specific materials used, their quality, and the design parameters.

The performance of this structure can be assessed by various factors:

1- Conversion Efficiency (η): This is a crucial metric, representing the percentage of sunlight that is converted into electricity. The choice of materials, layer thicknesses, and overall design will influence the conversion efficiency.

2- The fill factor (FF) is a measurement of solar cell effective converts sunlight into current. A higher fill factor indicates more efficient energy conversion.

3- The short circuit current Density (Jsc) is measuring the maximum current can produce under short-circuit conditions. It's influenced by the materials and their ability to absorb and convert photons into current.

4- The open circuit voltage (Voc) is representing the maximum voltage the cell can produce when there's no external load. It's determined by the material properties and the bandgap of the absorber layer (Sb_2S_3).

5- Quantum Efficiency (Q.E): Q.E is a measure of how well the solar cell responds to light of different wavelengths. It can reveal the effectiveness of the layers in capturing and converting specific wavelengths of light.

6- Thickness and Material Properties: The thickness of each layer, as well as the specific material properties, play a significant role in the performance of the solar cell. Adjusting these parameters can optimize the cell's efficiency.

Understanding the relationships between current, voltage, efficiency, and key parameters like Jsc, Voc, and J_0 is essential for solar cell development and analysis. The equations below describe key parameters and relationships in the operation of a solar cell. Here's an overview of these equations [15]:

The current-voltage relationship in a solar cell is crucial for understanding its behavior. Equation (1) defines the total current, J(V), which is the difference between the short-circuit

Equation (2) describes the dark current, which is the current that flows when there's no light. It's influenced by the saturation current, J0, and temperature (T).

$$J_{dark}(V) = J_0\left(\boldsymbol{e}^{qv/\kappa_{BT}} - 1\right) \qquad \dots \dots (2)$$

Equation (3) combines Jsc and J_dark to provide a more complete picture of the current-voltage relationship in the solar cell. This equation accounts for the impact of both light-generated current and dark current on the total current output.

$$J(V) = J_{SC} - J_0 \left(e^{\sqrt[q]{k_B T}} - 1 \right) \qquad \dots \dots (3)$$

Equation (4) expresses total current, J(V), and dark current, J0. It helps analyze how Jsc changes with varying voltage across the solar cell.

$$J_{SC} = J(V) + J_0 \left(e^{\frac{qv}{\kappa_{BT}}} - 1 \right) \qquad \dots \dots \dots (4)$$

Equation (5) defines the open circuit voltage, Voc when the terminals are not connected. It depends on the thermal voltage (K_B T/q), the optical current density (Jph), and J_0 .

$$V_{OC} = (K_B T / q) ln(J_{Ph} / J_0 + 1) \qquad \dots \dots (5)$$

Equation (6) relates the maximum power (P_max) generated by the solar cell to Jsc, Voc, and the current (Jmp) and voltage (Vmp) at the point of maximum power. FF is a measure of how well the solar cell utilizes its current and voltage to maximize power output.

$$FF = (J_{mp} \times V_{mp}) / (V_{OC} J_{SC}) = (P_{max}) / V_{OC} J_{SC} \qquad \dots \dots (6)$$

Equation (7) calculates the conversion efficiency of the solar cell, representing the ratio of the maximum power generated (P_max) to the incident power (Pin). The incident power is usually 1000 W/m^2 for solar cells under standard conditions (AM 1.5).

3.1. Adding And Replacing Adjustment Layers

In photovoltaic cells, the matching layer, often referred to as the buffer or window layer, plays a crucial role in facilitating the efficient interaction between the incident light and the absorption layer so that the largest possible amount of light reaches the absorption layer [16],[17], so it is necessary to obtain in this layer the least losses in absorption and be able to output the carriers of the optical current. Obtained using the lowest recombination losses, the presence of a large energy gap in the matching layer is very necessary in order to allow the largest number of carriers to pass through the absorption layer. Therefore, we find it necessary to improve the alignment layer because it is aligned with the energy gap between (Sb₂S₃) and the window (ZnO). In this part we used materials in the sequence (TiO₂, CdS, V₂O₅, Cdo, ZnSe) with an energy gap ranging between (2.28 - 3.56).

The compound cadmium sulfide (CdS) was chosen as the best compatible layer to improve the interface layer (Sb₂S₃), as it has higher current within the short-wavelength, has an energy gap of up to (2.4ev), and absorbs photons with (590 nm), which constitutes 24% of the total spectrum [18]. Therefore, it is considered a transparent layer wavelength more than (600 nm), which covers the largest part of spectrum and allows the highest light absorption in the absorption layer. It has distinctive electrical properties and optical transmittance, so it becomes a good layer in the

manufacture of solar cells [19]. There was an increase in open circuit voltage (Voc) and short circuit current density (Jsc), as well as conversion efficiency and fill factor when using the best layer among the layers. Table 1 and Table 2 shows the photocell outputs for each matching layer and parameters of materials used as matching layers respectively.

Material	Jsc(mA/Cm2)	Voc(v)	F.F. (%)	η(%)
Tio ₂	22.06	1.06	85.69	20.11
V_2O_5	22.08	1.06	87.35	20.53
CdO	22.05	1.1	78.44	19.04
ZnSe	22.10	1.06	77.26	18.18
CdS	22.11	1.06	87.53	20.59

Table 1. Outputs of a solar cell in relation to the layer used.

Table 2. Parameters of	materials used	as matching	layers.
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Parameters	symbol (unit)		V_2O_5	Cd0	ZnSe	CdS
		[20]	[21]	[22]	[23]	[24]
Energy gap	Eg (ev)	3.26	2.3	2.28	2.9	2.4
Thickness	W(µm)	0.05	0.5	0.5	0.5	0.05
Affinity of Electron	χ (ev)	4.2	3.99	4.5	4.1	4.2
Dielectric permittivity	€r	10	4.28	5.3	10	9
CB effective DOS	N_C (cm ⁻³)	1e+21	2.2e+18	2.2e+18	1.8e+18	1e+18
VB effective DOS	$N_{\rm v}~({\rm cm}^{-3})$	1e+20	1.8e+19	1.8e+19	1.8e+19	1e+19
Velocity of thermal electron	$V_n(\text{cm/s})$	1e+7	1e+7	1e+7	1e+7	1e+7
velocity of thermal hole	$V_P(\mathbf{cm/s})$	1e+7	1e+7	1e+7	1e+7	1e+7
mobility of electron	μ_n (cm ² /v.s)	1e-3	1.26	e+21.460	1e+2	5e+1
Hole mobility	$\mu_p(cm^2/v.s)$	1e-3	e+13.450	e+13.950	e+22.5	2e+1
Shallow of donor density	$ND(1/cm^{3})$	1e+17	e+191	e+221	e+51	1e+17
Shallow of acceptor density	<i>NA</i> (1/cm ³)	0	0	0	0	0
Absorption coefficient	α (1/cm)	1e+5	1e+5	1e+5	1e+5	1e+5

When using the CdS layer in the structure, it indicates that there were improvements in the voltage-current characteristics (I/V curve) and the quantum efficiency (Q.E) of the cells after the enhancements. Figure 2 represents the I-V curve for the cells with the CdS layer. The good results in this curve suggest improved electrical performance. In Figure 3, the Q.E curve for the cells after the improvements is depicted. Quantum efficiency refers to the ability of a solar cell to convert incoming photons into electrical current.

The curve indicates a change in quantum efficiency over a specific range of wavelengths.

Where R_{λ} is the absorption coefficient from the upper surface and (λ) is the wavelength.

The change in the Q.E curve between approximately 375 nm and 540 nm is attributed to the energy gap values of the layers used which is confined between (2.28 - 3.56) electron volts, according to equation (8). The matching layer, in this case, CdS, has an energy gap that aligns well with this range of wavelengths.

The text mentions that the matching layer (CdS) can be considered a "window" for light with wavelengths greater than 540 nm. This means that the CdS layer allows the absorption of a significant number of photons reaching the absorption layer (Sb_2S_3), enhancing the cell's light absorption and, consequently, its overall efficiency as indicated by the I-V and Q.E curves.



Figure 2. Current/voltage characteristic for the used matching layers.



Figure 3. Quantitative efficiency curves for layers used as matching layers.

3.2. Effect Of Sb₂s₃ Thickness Absorption Layer

The provided information discusses the impact thickness of the (Sb_2S_3) absorption layer on the structure performance, especially when combined with the best reflection layer (CuSbS₃). Increasing the absorption layer thickness of the (Sb_2S_3) has a noticeable effect on various parameters of the solar cell. It's observed when increasing the absorption layer thickness, there is an increase in both the (Voc) and (Jcs). These are essential factors contributing to improved conversion efficiency [25] as shown in equation (5). The increase in conversion efficiency is attributed to the increased absorption rate [26]. Also, the absorption layer thickness is increase, it can capture more light, which leads to higher efficiency. However, there is a decrease in the fill factor. This is due to the series resistance, which is directly proportional to the thickness of the absorption layer. As thickness increases, the series resistance also increases, affecting the fill factor negatively [27] as in equation (6).

The study involved increasing the thickness of the absorption layer in increments, from 0.5 μ m to 4 μ m. It was found that the best thickness for the absorption layer is 4 μ m. At this thickness, the solar cell achieved a conversion efficiency of 23.21%.

Figure 4, illustrates the relationship between the thickness of the absorption layer and the I-V curve. This curve is essential for understanding the electrical behavior of the solar cell with varying thickness. Table 3 Provides a detailed breakdown of the solar cell's performance parameters at different thickness levels, allowing a comprehensive analysis of how these parameters change with thickness.

	1	0 1	1	
Thickness(µm)	VOC	Jsc	FF(%)	η(%)
0.5	1.06	17.78	87.6	16.56
1	1.06	22.11	87.5	20.59
1.5	1.06	23.58	87.51	21.96
2	1.06	24.2	87.51	22.55
2.5	1.06	24.52	87.51	22.85
3	1.06	24.7	87.51	23.03
3.5	1.06	24.81	87.52	23.14
4	1.06	24.89	87.53	23.21

Table 3. Solar cell outputs with increasing absorption layer thickness.





There is a close relationship between the absorption layer thickness and the quantum efficiency (Q.E) of the solar cell, particularly in the context of spectral response.

The absorption layer thickness has a significant impact on quantum efficiency. Quantum efficiency is not constant but varies with the incident light wavelength.

Recombination is one of the factors that can reduce quantum efficiency. When recombination occurs, charge carriers (electron-hole pairs) recombine instead of being collected and contributing to the electrical output of the solar cell. This is a loss mechanism. As shown in equation (9) which describes the relationship between quantum efficiency (Q.E) and spectral response, which relates how well the solar cell responds to different wavelengths of light.

At longer wavelengths, where the highest absorption of charge carriers occurs, the quantum efficiency is also at its highest. This indicates that the solar cell is most effective at converting longer-wavelength light into electrical energy.

Figure 5, Illustrates how quantum efficiency changes with increasing absorption layer thickness. The figure shows that the highest quantum efficiency is achieved when the absorption layer thickness is $4 \mu m$.

$$SR(\lambda) = 0.808 \lambda QE(\lambda) \qquad \dots \dots (9)$$

Wavelength: λ

Spectral response: $SR(\lambda)$

The impact of increasing the absorption layer thickness on the (FF).



Figure 5. Quantum Efficiency (Q.E) curve for the thickness effect on the absorption layer of a solar cell.

The results shown when the thickness of the absorption layer in a solar cell is increased, it can lead to several effects on the cell's performance.

One of the consequences of thicker absorption layers is the generation of grains within the material. These grains can create defects or irregularities in the material's structure.

As a result of the presence of grains, there can be an increase in interface current. Interface current refers to the charge flow of carriers (electrons and holes) across boundary between different materials within the solar cell.

The generation of grains and the increase in interface current can have negative effects on the fill factor. The (FF) is a critical parameter that indicates how effectively a solar cell converts light into electrical energy. Additionally, the increase in interface current can lead to a decrease in the current within the depletion region cell. The depletion region is a crucial part of the cell where carriers are separated and collected.

The energy levels for the best thickness were obtained in Figure 6.

All these factors, including the generation of grains, increased interface current, and reduced current in the depletion region, can collectively reduce the overall efficiency of the solar cell.



Figure 6. Energy levels of the best absorption layer thickness (Sb_2S_3) .

3.3. Effect of adding second absorption layers to the Sb₂S₃ solar cell

Reflection layers, particularly CuSbS₃ with a thickness of (0.05 μ m), were added to the cell, which contributed to improved efficiency. A matching layer, CdS with thickness of (0.05 μ m), was also introduced to enhance the interface between the absorption and reflection layers.

The thickness of the primary absorption layer, Sb_2S_3 , was varied to find the optimal thickness. After testing different thicknesses, the best performance was achieved at a thickness of 4 μ m, which resulted in increased conversion efficiency.

A secondary absorption layer was added between the reflection layer (CuSbS₃) and the primary absorption layer (Sb₂S₃). Various materials with energy gaps ranging between 1 to 1.5 electron volts (eV) were tested for this purpose, including MAPbI₃, Sb₂Se₃, CZTS, and CZTSe as shown in table 4.

Table 4. Output of the solar cen for various materials employed as absorption layers.							
Material	Jsc(mA/Cm ²)	Voc(v)	F.F.(%)	η(%)			
Original solar cell	24.18	1.06	87.52	23.14			
MAPbI ₃	25.34	1.01	85.39	22.04			
CZTS	25.42	1.03	85.48	22.52			
CZTSe	30.33	1.03	85.4	26.88			
$\mathbf{Sb}_2\mathbf{Se}_3$	31.23	1.01	85.12	27.01			

Table 4. Output of the solar cell for various materials employed as absorption layers.

The secondary absorption layer material that provided the highest conversion efficiency was identified as Sb₂Se₃, with a remarkable efficiency of 27.01%.

Table 5 contains the parameters of the materials used as absorption layers, which include details about their energy gaps and other characteristics.

Parameters	symbol (unit)	MAPbI ₃ [28]	CZTS [29]	CZTSe [30]	Sb ₂ Se ₃ [31]
Thickness	W(µm)	1	1	1	1
Energy gap	Eg (ev)	1.5	1.5	1	1.2
Affinity of electron	χ (ev)	3.93	4.3	4.35	4.04
Dielectric permittivity	€r	30	7	13.6	18
Conduction band effective DOS	$N_C \text{ (cm}^{-3})$	2.5e+20	2.2e+18	2.2e+18	2.2e+18
Valance band effective DOF	$N_{\rm v}~({\rm cm}^{-3})$	2.5e+20	1.8e+19	1.8e+19	1.8e+19
Velocity of thermal electron	$V_n(cm/s)$	1e+7	1e+7	1e+7	1e+7
Velocity of thermal Hole	$V_P(\mathbf{cm/s})$	1e+7	1e+7	1e+7	1e+7
Electron Mobility	μ_n (cm ² /v.s)	5e+1	5e+2	1e+2	1.5e+1
Hole Mobility	μ_p (cm ² /v.s)	5e+1	2.5e+1	2.5e+1	5.1e0
Density of Shallow donor	<i>ND</i> (1/cm ³)	0	0	0	0
Density of Shallow acceptor	<i>NA</i> (1/cm ³)	5e+18	5e+18	5e+18	5e+18
Absorption Coefficient	a (1/cm)	-	-	-	-

Table 5. Parameters of materials used as secondary absorption layers.

The figures and information provided highlight the improvements in the solar cell's performance after changing and adding absorption layers.

Figure 7, illustrates the impact on the current-voltage (I-V) curve by changing and adding absorption layers. A notable improvement is observed, suggesting enhanced electrical characteristics.

The quantitative efficiency (Q.E) curve shows significant enhancement, with the curve closely resembling an ideal square shape. This square-like curve represents an efficient utilization of incident light, making it closer to the ideal condition for quantum efficiency.

Figure 8 Illustrating how quantum efficiency changes with wavelength before and after adding absorption layers. This curve is essential for understanding how efficiently the solar cell converts photons at different wavelengths into electrical current. The figure demonstrates an improvement in quantum efficiency across a range of wavelengths following the addition of absorption layers. It's common for the Q.E curve to exhibit enhanced performance characteristics after optimizing the solar cell structure, indicating that more photons are being effectively converted into electricity. This is a key indicator of improved solar cell performance.

Figure 9, displays the energy levels of the (CB) and (VB) for the best absorption layer used in enhancing the solar cell, which is Sb_2Se_3 . This material, responsible for the improved quantum efficiency, is a pure layer acting as a selective barrier for electrons and holes. Noting that the conversion efficiency increased from (23.21%) to (27.01%). This selective barrier minimizes recombination possibilities and promotes carrier separation speed, similar to traditional P/N

solar cells. This positively impacts the solar cell's performance [32]. Table 6 shows comparing the cell outputs after adding reflection layers, particularly CuSbS₃, changing thickness of the primary absorption layer and adding secondary absorption layer.



Figure 7. Current/voltage characteristic curve of the original cell with the resulting cell after adding absorption layers.



Figure 8. Quantum efficiency curve Vs. wavelength before and after adding absorption layers.





Solar Energy and Sustainable Development, $V_{Olume}(13)$ - $\mathcal{N}(1)$. June 2024

Structure of solar Cell	Voc(V)	-Jsc (mA/cm ²)	F.F. (%)	η (%)
Original Cell "glass/Mo/Sb ₂ S ₃ /CdS/ i:ZnO/AL:ZnO"	0.996	18.74	61.2	11.43
"glass/Mo/CuSbS ₃ / Sb ₂ S ₃ /CdS/ i:ZnO/AL:ZnO"	1.06	22.11	87.53	20.59
Thickness "glass/Mo/CuSbS ₃ / Sb ₂ S ₃ /CdS/ i:ZnO/AL:ZnO"	1.06	24.89	87.53	23.21
"glass/Mo/CuSbS3/Sb2S3/ Sb2S3/ CdS/i:ZnO/AL:ZnO"	1.01	31.23	85.12	27.01

Table 6. Compares the cell outputs after implementing various improvements in the solar cell structure.

4. CONCLUSION

Increasing the original absorption layer thickness of the (Sb_2S_3) from 1 to 4 µm leads to a significant increase in the solar cell's conversion efficiency (η), with the efficiency reaching 23.21%. This suggests that carefully tuning the absorption layer thickness is crucial for maximizing solar cell performance.

By introducing Sb_2Se_3 as a secondary absorption layer between the original absorption layer (Sb_2S_3) with a thickness of 4 µm and the reflection layer, and by using the best-matching layer (CdS), the solar cell's efficiency significantly improved. The conversion efficiency reached 27.01%. This demonstrates that adding a second absorption layer enhances the cell's performance.

The most important conclusion in research highlights the importance of exploring effect of a secondary absorption layer on solar cell performance. In addition of this layer can lead to substantial improvements in conversion efficiency, making it a valuable component to study and integrate into solar cell designs.

These conclusions underscore the significance of thickness optimization and the potential benefits of incorporating additional absorption layers in solar cell structures. By carefully adjusting these parameters, researchers can continue to enhance solar cell efficiency, bringing us closer to more efficient and sustainable solar energy conversion.

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