Simulating the performance of a highly efficient CuBi_2O_4 -based thin-film solar cell

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Abstract

In this study, copper bismuth oxide (CuBi_2O_4) absorber-based thin film heterojunction solar cell structure consisting of $\text{Al}/\text{FTO}/\text{CdS}/\text{CuBi}_2\text{O}_4/\text{Ni}$ has been proposed. The proposed solar cell device structure has been modeled and analyzed by using the solar cell capacitance simulator in one dimension (SCAPS-1D) software program. The performance of the proposed photovoltaic device is evaluated numerically by varying thickness, doping concentrations, defect density, operating temperature, back metal contact work function, series and shunt resistances. The current density–voltage behaviors at dark and under illumination are investigated. To realize the high efficiency CuBi_2O_4 -based solar cell, the thickness, acceptor and donor densities, defect densities of different layers have been optimized. The present work reveals that the power conversion efficiency can be enhanced by increasing the absorber layer thickness. The efficiency of 26.0% with open-circuit voltage of 0.97 V, short-circuit current density of $31.61 \text{ mA}/\text{cm}^2$, and fill-factor of 84.58% is achieved for the proposed solar cell at the optimum $2.0\text{-}\mu\text{m}$ -thick CuBi_2O_4 absorber layer. It is suggested that the p-type CuBi_2O_4 material proposed in the present study can be employed as a promising absorber layer for applications in the low cost and high efficiency thin-film solar cells.

Keywords Thin-film solar cell · CuBi_2O_4 absorber · CdS buffer · SCAPS-1D · Efficiency

1 Introduction

Thin-film solar cells (TFSCs) utilizing semiconducting absorber materials, such as CdTe, CIGS etc., have received as the most promising candidate for the photovoltaic device applications due to its high efficiency and compatible with the fabrication process [1–6]. However, the conventional absorber materials in the TFSCs still face some challenges such as scarcity of materials, high cost of materials processing, and device fabrication steps limiting the implementation of solar electricity on large scales. Although considerable numbers of studies have been conducted to explore alternative absorber materials in

the TFSCs, unfortunately, no works have been successful in replacing the ordinary materials [7–10].

In recent years, copper (Cu)-based ternary oxide semiconductors with narrow energy band gaps have been attracted significant attention as a photocathode material for solar energy conversion [11, 12]. Particularly, p-type CuBi_2O_4 has been taken as one of the most encouraging photocathode material due to low cost and easily processable for the solar cell technology [13–15]. The advantages of CuBi_2O_4 are narrow energy band gap from 1.4 to 1.8 eV [13–17], which is near the optimum value for solar cell applications, high optical absorption coefficient exceeding 10^4 cm^{-1} [15, 17], non-toxicity, and sufficient resource. In CuBi_2O_4 material, Cu is a chemical element having atomic number 29, group 11,

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period 4, which is a soft, malleable, and ductile metal with very high thermal and electrical conductivity [18]. No other metal is verified to be more naturally diamagnetic than bismuth. Bismuth (Bi) is a soft, crystalline, brittle silvery metal having lower thermal conductivity. It is stable to oxygen and water. The atomic number of bismuth is 83, group 15 [19]. Oxygen (O) is a colorless nonmetallic chemical element of the periodic table [20]. Oxygen has reactivity which can be produced by electric discharge in oxygen or by the action of ultraviolet radiation on oxygen in the stratosphere. Oxygen is a strong oxidizing agent and has the second highest electronegativity of all reactive elements [20].

Several heterojunction architectures based on the CuBi_2O_4 materials have been investigated in the previous studies [13, 16, 21–26]. The photocatalytic performances have studied for the p–n heterojunction structures with $\text{CuBi}_2\text{O}_4/\text{WO}_3$ [13, 21], $\text{CuBi}_2\text{O}_4/\text{CeO}_2$ [16], $\text{CuBi}_2\text{O}_4/\text{SnO}_2$ [22], $\text{CuBi}_2\text{O}_4/\text{g-C}_3\text{N}_4$ [23], $\text{CuBi}_2\text{O}_4/\text{NiO}$ [24], and $\text{CuBi}_2\text{O}_4/\text{CuO}$ [25, 26] fabricated by hydrothermal synthesis and pulsed laser deposition processes. In addition, high-density p-type CuBi_2O_4 thin-film on FTO glass substrate is fabricated by spin-coating process for solar applications [27]. Thus, the thin-film of ternary oxide semiconductor CuBi_2O_4 is expected to be utilized as one of the most prospective absorber materials in the TFSCs due to its high absorption coefficient, narrow energy band gap, and nontoxicity. Moreover, the thin-films of CuBi_2O_4 material in the heterojunction structures can be fabricated by the solution processes, which would be very effective for cost-effective and high performance light harnessing elements comparing the conventional absorber materials. However, there are few reports on the CuBi_2O_4 -based thin-film solar cell with poor light conversion efficiency [28]. Therefore, a new type of thin-film heterojunction solar cell with sufficient photovoltaic performances employing the CuBi_2O_4 material as an absorber layer is expected to be explored. Hence, it is necessary to understand the transport of photo-generated charge carriers in the CuBi_2O_4 -based thin-film heterojunction devices.

In order to realize the CuBi_2O_4 -based TFSC, in the present study, an effective heterojunction architecture with $\text{Al}/\text{SnO}_2:\text{F}(\text{FTO})/\text{CdS}/\text{CuBi}_2\text{O}_4/\text{Ni}$ is designed for the first time. The SCAPS-1D simulator is used to investigate the performance parameters such as open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill-factor (FF), and efficiency (η) of the proposed CuBi_2O_4 -based TFSC.

2 Device and simulation

In this work, the novel heterojunction solar structure $\text{Al}/\text{FTO}/\text{n-CdS}/\text{p-CuBi}_2\text{O}_4/\text{Ni}$ is designed and simulated by the SCAPS-1D software program [29]. Figure 1 illustrates the

schematic diagram of the proposed CuBi_2O_4 -based TFSC. In the proposed heterojunction structure, mostly used n-type CdS is employed as a buffer layer to couple with the p-type CuBi_2O_4 absorber layer in the solar cell. Also, the window layer of fluorine doped tin oxide $\text{SnO}_2:\text{F}$ (FTO) is introduced. This simulation software developed by the Department of Electronics and Information Systems, University of Gent is useful to design and simulate the TFSCs with different layered structures, as shown in Fig. 1. The energy band diagram of CuBi_2O_4 -based solar cell is illustrated in Fig. 2. The energy band gaps and thicknesses of CuBi_2O_4 , CdS buffer, and FTO window layers are indicated in Fig. 2. In this simulation, the detailed investigations of the proposed solar cell by changing various parameters [9–11, 16, 23, 30–35, 39] summarized in Table 1 have been executed using the SCAPS-1D. The photovoltaic performance parameters such as V_{oc} , J_{sc} , FF, and η are measured using the simulation tool. The designed CuBi_2O_4 -based thin-film solar structure is illuminated under AM1.5G solar spectrum with $100 \text{ mW}/\text{cm}^2$ incident power density. The value of the absorption coefficient, (cm^{-1}), as a function of the wavelength, (nm), for the CuBi_2O_4 thin-film material is taken from experimental result reported in previous work [33], on the other hand, the absorption files for the n-type CdS buffer and FTO window layers are used from the SCAPS simulation program [29]. The work function values of 4.28 eV [38] and 5.15 eV [38] are employed for the aluminum (Al) as front contact and nickel (Ni) as back contact, respectively. The thermal velocity of $1 \times 10^7 \text{ cm/s}$ for electrons and holes in each layer has been put during

Fig. 1 Schematic diagram of the proposed structure of CuBi_2O_4 -based TFSC

Fig. 2 Energy band diagram of CuBi₂O₄-based solar cell

the simulation work [37, 39]. The surface recombination velocities for both electrons and holes are set to 10^7 and 10^5 cm/s at front contact and 10^5 and 10^7 cm/s at back contact, respectively [36, 39]. The parameters utilized at the CdS/CuBi₂O₄ interface for the simulation study are illustrated in Table 2.

3 Results and discussion

In the present work, CuBi₂O₄-based TFSC has been investigated by the SCAPS-1D software. The structure depicted in Fig. 1 is simulated with the depth of the layers according to the sunlight illumination. Figure 3 represents the current density–voltage (J–V) characteristics of the CuBi₂O₄-based solar cell at dark and under

Table 2 Interface parameters used in the Al/FTO/n-CdS/p-CuBi₂O₄/Ni heterojunction device simulation

Parameters (unit)	CdS/CuBi ₂ O ₄ interface
Defect type	Neutral
Capture cross-section of electrons (cm ²)	1×10^{-18}
Capture cross-section of holes (cm ²)	1×10^{-18}
Reference for defect energy level	Above the highest E _v
Energy with respect to reference (eV)	0.1
Total density (cm ⁻²)	1×10^{10}

illumination conditions. The thicknesses of 2.0 μm, 0.06 μm, and 0.05 μm are employed for the CuBi₂O₄, CdS, and FTO, respectively. Typical Schottky diode behavior is observed in the J–V curve at the dark condition. It can also be seen that the application of light on the heterojunction device results in the increasing of current density up to 31.61 mA/cm². The photo-generated electrons and holes are increased with increasing the incident photons. This leads to suggest that the absorption of the charge carriers in the CuBi₂O₄ layer would be enhanced, and hence improve the performance of the solar cell. Figure 4 demonstrates the quantum efficiency of the CuBi₂O₄-based solar cell with varying the absorber thickness as a function of the wavelength. Here, the quantum efficiency is defined as the ratio of the number of carriers collected by the solar cell to the number of photons of a given energy incident on the solar cell. The thickness of the CuBi₂O₄ absorber layer is varied from 1.0 to 3.0 μm, while keeping the thicknesses of the CdS and the FTO are fixed at 0.06 μm and 0.05 μm, respectively. It can be found that the quantum efficiency increases at longer wavelength as the increase of the absorber thickness, as

Table 1 Summary of the simulation parameters for different materials

Parameters (unit)	Absorber (p-CuBi ₂ O ₄)	Buffer (n-CdS)	Window (SnO ₂ :F)
Thickness (nm)	2000*	60*	50*
Band gap (eV)	1.5 [14, 30, 33]	2.4 [34]	3.6 [36, 37]
Electron affinity (eV)	3.72 [31]	4.2 [34, 35]	4 [36, 37]
Dielectric Permittivity	34 [30]	10 [34]	9 [36, 37]
CB effective DOS (cm ⁻³)	1.2×10^{19} [30, 32]	2.2×10^{18} [34]	2.2×10^{18} [36, 37]
VB effective DOS (cm ⁻³)	5×10^{19} [16, 30, 33]	1.8×10^{19} [34]	1.8×10^{19} [36, 37]
Electron mobility (cm ² V ⁻¹ s ⁻¹)	1.1×10^{-3} [16, 30, 33]	100 [34, 35]	100 [36, 37]
Hole mobility (cm ² V ⁻¹ s ⁻¹)	1.2×10^{-3} [16, 23, 30]	25 [34, 35]	25 [36, 37]
Donor density, N _D (cm ⁻³)	0	1×10^{17} [35]	1×10^{18}
Acceptor density, N _A (cm ⁻³)	3.7×10^{18} * [30]	0	0
Defect type	SD	SA	–
Energy distribution	Gaussian	Gaussian	–
Bulk defect density (cm ⁻³)	1×10^{12} *	1×10^{14} *	–

N.B. *is a variable field

CB conduction band, VB valence band, DOS density of states, SA single-acceptor, SD single-donor

Fig. 3 J–V characteristics of the CuBi₂O₄-based solar cell at the dark and under illumination

Fig. 4 Quantum efficiency of the CuBi₂O₄-based solar cell with varying the absorber thickness as a function of the wavelength

shown in Fig. 4. It is thus suggested that the absorption of photons would be increased as the increase of the absorber thickness at the higher wavelength.

3.1 Effects of thickness and donor density of window layer on cell performances

In the designed heterojunction TFSC, a transparent conductive oxide, namely, FTO as the window layer is

employed. The output parameters of the CuBi₂O₄-based solar cell are evaluated by varying the window layer thickness ranged from 10 to 200 nm, as exhibited in Fig. 5a. The thicknesses of the CuBi₂O₄ and CdS are kept constant at the optimized values of 2000 nm and 60 nm, respectively. The simulated results show that all the solar cell output parameters are almost stable at the FTO thickness less than 100 nm. In addition, it is found that the photo-generated current is minimized a bit at the thicker FTO, and hence reduced the overall performances lightly. This result is due to the less photon reached to the absorber through the thicker window layer. Thus, the window layer thickness is preferred to be 50 nm taking into account of the overall performances.

In this numerical study, the donor density of FTO is changed from 1×10^{14} to $5 \times 10^{20} \text{ cm}^{-3}$ with 2000-nm-absorber (acceptor density of $3.7 \times 10^{18} \text{ cm}^{-3}$), 60-nm-buffer (donor density of $1 \times 10^{17} \text{ cm}^{-3}$) and 50-nm-window. Figure 5b shows the effect of the donor density on the photovoltaic performances parameters such as V_{oc} , J_{sc} , FF, and η of the proposed TFSC. It can be observed that V_{oc} , J_{sc} , FF, and η are approximately similar with increasing the window layer donor density. η of the proposed CuBi₂O₄-based solar cell is obtained about 26% at the donor density ranged from 1×10^{14} to $5 \times 10^{20} \text{ cm}^{-3}$. In this work, the FTO donor density has been picked to be $1 \times 10^{18} \text{ cm}^{-3}$ considering low cost of the solar cell fabrication.

3.2 Effects of thickness and donor density of buffer layer on cell performances

Figure 6a shows the effect of the buffer layer thickness on the CuBi₂O₄ solar cell output parameters. To optimize the performance of the CuBi₂O₄-based TFSC, the thickness of the CdS buffer layer is changed from 40 to 100 nm, while the thicknesses of the absorber ($N_A = 3.7 \times 10^{18} \text{ cm}^{-3}$) and the window ($N_D = 1 \times 10^{18} \text{ cm}^{-3}$) layers are set constant at 2000 nm and 50 nm, respectively. In Fig. 6a, it can be observed that the solar cell output parameters such as V_{oc} , J_{sc} , FF, and η are almost constant as the function of the CdS buffer layer thickness. This is due to insufficient electron–hole pairs produced in the CuBi₂O₄ absorber layer. It is suggested that a smaller quantity of lights will come to the absorber through the thicker buffer layer, and hence resulted the insignificant current for inadequate photo-generated electrons and holes. Therefore, a thin buffer layer is anticipated to achieve outstanding solar cell performances. The optimum thickness of the buffer layer is selected to be 60 nm for the following calculations in this simulation work, which is consistent with the buffer thickness employed in the previous works [37, 39, 40].

Fig. 5 Photovoltaic performance parameters such as V_{oc} , J_{sc} , FF, and η of the proposed CuBi₂O₄-based solar cell by varying the **a** thickness and **b** donor density of the window layer

In this simulation, the effect of the CdS donor density ranging from 1×10^{12} to 5×10^{18} cm⁻³ with 2000-nm-thick absorber (acceptor density of 3.7×10^{18} cm⁻³), 60-nm-CdS, and 50-nm-FTO (donor density of 1×10^{18} cm⁻³) is analyzed. Figure 6b manifests the performance parameters such as V_{oc} , J_{sc} , FF, and η of the CuBi₂O₄-based TFSC as a function of the donor density of buffer layer. It is seen that all the output characteristics of the proposed solar cell are almost constant up to the density of 1×10^{17} cm⁻³. Beyond this density, the performance parameters are changed slowly with increasing the donor density of CdS. In the present study, the optimum doping concentration in the CdS buffer is evaluated to be 1×10^{17} cm⁻³. At the density of 1×10^{17} cm⁻³, η of 26.0% with V_{oc} of 0.97 V, J_{sc} of 31.62 mA/cm², and FF of 84.58% is estimated.

3.3 Effects of thickness and acceptor density of absorber layer on cell performances

The solar cell performances such as V_{oc} , J_{sc} , FF, and η are analyzed by varying the CuBi₂O₄ absorber thickness, as depicted in Fig. 7a. The thickness of absorber ($N_A = 3.7 \times 10^{18}$ cm⁻³) are changed from 100 to 3000 nm, while thicknesses of CdS ($N_D = 1 \times 10^{17}$ cm⁻³) and FTO ($N_D = 1 \times 10^{18}$ cm⁻³) are kept constant at 60 nm and 50 nm, respectively. In Fig. 7a, it can be obtained that V_{oc} increases from 0.92 to 0.98 V with increasing absorber thickness from 100 to 3000 nm. J_{sc} also increases as a function of the CuBi₂O₄ thickness. The values of J_{sc} at 100 nm and 3000 nm are estimated to be 7.45 mA/cm² and 35.26 mA/cm². The absorption of photons at the thicker absorber layer leads to increase the J_{sc} . It is also found that FF is increased for the CuBi₂O₄ thickness up to 400 nm and then reduced slightly for further increasing the thickness. This decreasing in FF is due to increase of series resistance. The

Fig. 6 Effects of **a** the thickness and **b** the donor density of the buffer layer on the performance parameters of the proposed solar cell

conversion efficiency, η , is boosted acutely from 5.83 to 26.0% with the thickness increased from 100 to 2000 nm, and then is enhanced moderately till the 3000-nm-thick CuBi_2O_4 absorber layer. It is suggested that the photo-generated electrons and holes will be increased greatly at thicker absorber layer and thus improved the overall performances of the solar cell. Therefore, in this study, the CuBi_2O_4 absorber thickness is optimized to be 2000 nm by taking into consideration the device fabrication cost, which would be selected as the optimum thickness for the further investigation.

The effect of the acceptor density of the absorber layer on the behavior of the CuBi_2O_4 solar cell performances is investigated in this study, as displayed in Fig. 7b. The acceptor density is varied from 3.7×10^{14} to 5×10^{19} cm⁻³, while the donor densities in the CdS and the FTO layers are set fixed at 1×10^{17} cm⁻³ and 1×10^{18} cm⁻³, respectively. It can be observed in Fig. 7b that V_{oc} is increased hardly up to 5.0×10^{18} cm⁻³, and then is raised greatly. The values of V_{oc} at 3.7×10^{14} cm⁻³ and 5.0×10^{19} cm⁻³ are found to be 0.97 V

and 1.02 V, respectively. J_{sc} is incremented from 34.56 to 43.98 mA/cm² till 3.7×10^{16} cm⁻³ and then is declined notably with increasing the hole density. The increase of the hole doping in the range from 3.7×10^{16} to 5.0×10^{19} cm⁻³ may lead to minimize the space charge width, and thus reduced carrier collection at the junction. FF is varied lightly up to 5.0×10^{16} cm⁻³ and then is enlarged linearly. The conversion efficiency is increased gradually from 19.85 to 26.0% till the acceptor density of 3.7×10^{18} cm⁻³. It is also found that the efficiency beyond the hole doping of 3.7×10^{18} cm⁻³ is not progressed importantly. Therefore, the acceptor density of the CuBi_2O_4 absorber for the proposed solar cell is chosen to be 3.7×10^{18} cm⁻³ in the interest of the cost and production rate of device fabrication.

3.4 Effect of bulk defect density in absorber and buffer layers on cell performances

Here, the effect of single donor like bulk defect density in the CuBi_2O_4 absorber on the cell performances is investigated,

Fig. 7 Solar cell performances such as V_{oc} , J_{sc} , FF, and η by varying **a** the thickness and **b** the acceptor density of the CuBi_2O_4 absorber layer

as revealed in Fig. 8a. The defect density of CuBi_2O_4 layer is varied from 1×10^{12} to $5 \times 10^{16} \text{ cm}^{-3}$ with the fixed CdS defect density of $1 \times 10^{14} \text{ cm}^{-3}$. In Fig. 8a, V_{oc} , J_{sc} , and η are decreased extremely with increasing the bulk defect density. This result is due to the high recombination rate of the charge carriers at the large defect density in the absorber. However, FF is changed moderately as a function of the CuBi_2O_4 defect density. The conversion efficiency for the CuBi_2O_4 defect density ranged from 1×10^{12} to $5 \times 10^{16} \text{ cm}^{-3}$ is estimated to be 26.0% and 3.09%, respectively.

Figure 8b shows the performances of the solar cell by varying the single acceptor like bulk defect density from 1×10^{12} to $5 \times 10^{16} \text{ cm}^{-3}$ in the CdS buffer. It can be seen that the output parameters such as V_{oc} , J_{sc} , FF, and η of the proposed CuBi_2O_4 -based solar cell are almost constant with the increasing of the CdS defect density. The efficiency from 26 to 25.87% with V_{oc} of 0.972 V, J_{sc} from 31.61 to 31.60 mA/cm^2 and FF from 84.58 to 84.25% is calculated for the CdS defect density in the range defined in Fig. 8b.

3.5 Effects of operating temperature and back contact metal work function on cell performances

In the present study, the impact of the operating temperature ranging from 273 to 473 K is evaluated to understand the performance and stability of the proposed solar cell. Figure 9a reports the variations in the performance parameters such as V_{oc} , J_{sc} , FF, and η of the proposed CuBi_2O_4 -based solar cell as a function of the operating temperature. As can be observed in the figure, V_{oc} , FF, and η are decreased with increasing the operating temperature. The value of V_{oc} at 273 K is determined to be 0.985 V and is declined to 0.876 V at 473 K. The drop of V_{oc} is due to the reduction of the energy band gap of the semiconductors with boosting the temperature. It can be also seen that J_{sc} is increased with expanding the temperature. The shift in energy band gap with the operating temperature results in the change of J_{sc} with the temperatures [41].

Fig. 8 Effect of bulk defect density in **a** the CuBi $_2$ O $_4$ absorber and **b** the CdS buffer layers on the cell performances

Typically, the energy band gap of most semiconductors reduces with increasing the operating temperature [41, 42]. These results are in good agreement with the behaviors of the temperature dependent photovoltaic performances reported by other authors [43]. In Fig. 9a, the degradation of V_{oc} contributes to the decrease in FF from 85.66 to 77.52% with the operating temperature varied from 273 to 473 K [43, 44]. These V_{oc} , J_{sc} and FF values are used to compute the maximum conversion efficiency of the solar cell using the equation found in Ref. [43]. The efficiencies of 26.61% and 21.68% are estimated at 273 K and 473 K, respectively. This reduction in conversion efficiency with the operating temperature is due to the decrease in V_{oc} and FF.

In this simulation work, the influence of the back contact metal work function on the device performance is also studied. The performance parameters such as V_{oc} , J_{sc} , FF, and η of the proposed solar cell is evaluated by varying the back contact metal work function, as illustrated in Fig. 9b. The work function of the back metal contact is shifted from 4.6 to 5.2 eV. It can be observed

that the V_{oc} , FF, and η increase significantly with increasing the work function up to 5.0 eV, and then are saturated. This leads to suggest that the barrier height of minority carrier could be minimized with the higher work function. It can also be found that the J_{sc} is almost fixed with the work function in the range defined in Fig. 9b. Similar behavior is also observed in the previous report [45]. It is revealed that the power conversion efficiency is greatly affected at the back contact metal work function ≤ 5.0 eV. Therefore, the back contact metal with work function greater than 5.0 eV (such as Au, Ir, Ni and Pd) should be selected to obtain the excellent photovoltaic performances. In this work, the metal Ni as a back contact material with the work function of 5.15 eV [38] is employed to achieve the high performance of CuBi $_2$ O $_4$ -based solar cell.

Fig. 9 Variations in the performance parameters such as V_{oc} , J_{sc} , FF, and η of the proposed CuBi₂O₄-based solar cell as a function of **a** the operating temperature and **b** the back contact metal work function

3.6 Effects of series and shunt resistances on cell performances

The series (R_s) and shunt (R_{sh}) resistances are important parameters to understand the device performance. In the present study, the influences of series and shunt resistances on the cell of performances of the CuBi₂O₄-based solar cell are simulated by varying R_s from 0 to 5 $\Omega\text{-cm}^2$ and R_{sh} from 50 to $10^7 \Omega\text{-cm}^2$. Figure 10a represents the cell performances such as V_{oc} , J_{sc} , FF, and η as a function of R_s . Here, the R_{sh} is fixed at $10^5 \Omega\text{-cm}^2$. As can be seen in the Fig. 10a, V_{oc} and J_{sc} are not changed notably with the R_s . It is also seen that FF and η are decreased considerably with the increase of R_s . These results obtained in this simulation are consistent with the findings reported in previous studies [42, 46]. The efficiencies of the proposed solar cell are calculated to be 25.99% and 21.4% for the R_s at 0 $\Omega\text{-cm}^2$ and 6 $\Omega\text{-cm}^2$, respectively. Figure 10b reveals the J–V behaviors of the proposed cell for various R_s . The J–V characteristics changes with varying the R_s . It is suggested

that the solar cell output parameters are influenced by increasing the R_s .

Figure 11a represents the solar cell performances as a function of the R_{sh} . In this case, the R_s is kept constant at 0.05 $\Omega\text{-cm}^2$. It can be found that the cell characteristics are shifted greatly up to the R_{sh} of $10^3 \Omega\text{-cm}^2$ and then are almost saturated with the R_{sh} higher than $10^3 \Omega\text{-cm}^2$. The simulated efficiency enhances from 18.88 to 25.95% for the R_{sh} shifted from 10^2 to $10^7 \Omega\text{-cm}^2$. The impact of R_{sh} on the J–V characteristics of proposed CuBi₂O₄-based TFSC is also demonstrated in Fig. 11b. These results imply that the series and shunt resistances have important effect on the performances of the photovoltaic devices.

4 Conclusions

In this study, a p-type CuBi₂O₄ material as the absorber layer with the n-CdS buffer layer in the thin-film heterojunction solar cell has been proposed for the first time.

Fig. 10 **a** Effect of R_s on the performance parameters of the proposed CuBi_2O_4 -based TFSC. **b** Effect of R_s on the J-V characteristics of the proposed cell

The SCAPS-1D simulation software program has been carried out to realize the designed heterojunction photovoltaic structure of $\text{Al/FTO/CdS/CuBi}_2\text{O}_4/\text{Ni}$. The effects of thickness, doping concentration, defect density, operating temperature, series and shunt resistances, and work function of back contact metal on the solar cell performances are analyzed extensively using the simulation tool. It is also found that the power conversion efficiency of the designed novel heterojunction structure is enhanced with increasing the CuBi_2O_4 absorber layer thickness. The optimum thicknesses of 2.0 μm , 0.06 μm , and 0.05 μm are found for the CuBi_2O_4 , CdS, and FTO, respectively. The open-circuit voltage, short-circuit current density, fill-factor, and efficiency are measured to be

0.97 V, 31.61 mA/cm^2 , 84.58% and 26.0%, respectively, at the optimized thicknesses. The doping concentrations of the absorber, buffer, and window layers are chosen to be $3.7 \times 10^{18} \text{ cm}^{-3}$, $1 \times 10^{17} \text{ cm}^{-3}$ and $1 \times 10^{18} \text{ cm}^{-3}$, respectively. To achieve the excellent performances, the defect densities of $1 \times 10^{12} \text{ cm}^{-3}$ and $1 \times 10^{14} \text{ cm}^{-3}$ are employed for the CuBi_2O_4 absorber and the CdS buffer layers, respectively. In addition, the temperature dependence performance parameters have been explored for the proposed CuBi_2O_4 -based solar cell. These results lead to suggest that the p-type CuBi_2O_4 material can be utilized as a potential absorber layer for the application in the highly efficient thin-film heterojunction solar cell.

Fig. 11 **a** Effect of R_{sh} on the performance parameters of the proposed CuBi_2O_4 -based TFSC. **b** Effect of R_{sh} on the J–V curve of the proposed solar cell

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Declarations

Conflict of interest The authors declare no conflict of interests.

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