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Enhancing Sb_2Se_3 thin-film solar cell efficiency via CuGaSe_2 dual-absorber integration

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Antimony selenide (Sb_2Se_3) thin-film solar cells have attracted considerable attention due to their earth-abundant composition, suitable bandgap, and high absorption coefficient. However, their performance remains limited by carrier recombination, interfacial losses, and incomplete spectral utilization. In this work, a CuGaSe_2 -assisted dual-absorber architecture is proposed and investigated using SCAPS-1D simulation to enhance the optoelectronic performance of Sb_2Se_3 -based solar cells. The reference structure ($\text{Mo}/\text{MoSe}_2/\text{Sb}_2\text{Se}_3/\text{CdS}/\text{ZnO}/\text{Al}/\text{ZnO}$) is first calibrated against experimental data, showing excellent agreement in key photovoltaic parameters. A CuGaSe_2 layer is then introduced between Sb_2Se_3 and CdS , forming a $\text{Mo}/\text{MoSe}_2/\text{Sb}_2\text{Se}_3/\text{CdS}/\text{ZnO}/\text{Al}/\text{ZnO}$ heterostructure. The proposed device exhibits a significant improvement in performance, with power conversion efficiency increasing from 10.12 to 19.50%, accompanied by an increase in open-circuit voltage from 0.48 to 0.77 V and short-circuit current density from 30.87 to 35.80 mA cm^{-2} . This enhancement is attributed to improved optical utilization, enhanced carrier generation, and suppressed recombination losses associated with favorable band alignment and modified interfacial energetics introduced by the CuGaSe_2 layer. Additional analyses reveal an increase in built-in potential and a reduction in recombination activity compared with the reference device. Overall, these results demonstrate that CuGaSe_2 can play a beneficial dual role as both an auxiliary absorber and an interfacial energy-modulating layer in Sb_2Se_3 -based thin-film solar cells.

Keywords Sb_2Se_3 solar cells, CuGaSe_2 secondary absorber, Dual-absorber heterostructure, SCAPS-1D simulation, Recombination dynamics

Thin-film photovoltaic technologies are of continuing interest because they reduce material consumption, enable lightweight and flexible device architectures, and allow device-level bandgap and interface engineering. Among emerging inorganic chalcogenides, antimony-based absorbers have attracted particular attention because of their earth-abundant composition, strong optical absorption, and potential compatibility with scalable deposition methods^{1–10}.

Among these materials, antimony selenide (Sb_2Se_3) has emerged as one of the most attractive candidates for next-generation thin-film photovoltaics. Related antimony chalcogenides such as Sb_2S_3 typically exhibit a wider bandgap of approximately 1.7–1.8 eV and a high optical absorption coefficient above 10^4 cm^{-1} , making them promising wide-bandgap absorbers for thin-film photovoltaic applications¹¹. In contrast, Sb_2Se_3 possesses a narrower optical bandgap of approximately 1.1–1.3 eV and a high absorption coefficient exceeding 10^5 cm^{-1} in the visible region, enabling efficient broadband light harvesting using micrometer-scale absorber thicknesses^{1,4,8}. In addition, the binary composition of Sb_2Se_3 avoids the complex multicomponent phase control often encountered in kesterite and chalcopyrite absorbers. These characteristics make Sb_2Se_3 a promising platform for low-cost, stable, and resource-conscious photovoltaic devices^{12–14}.

The anisotropic crystal structure of Sb_2Se_3 further complicates carrier transport. Sb_2Se_3 consists of quasi-one-dimensional $[\text{Sb}_4\text{Se}_6]_n$ ribbons, and the orientation of these ribbons relative to the substrate plays a crucial role in determining carrier transport pathways. Favorable ribbon orientation can facilitate carrier extraction, whereas unfavorable orientation may increase transport resistance and recombination losses. Consequently, device optimization requires simultaneous control over absorber thickness, defect density, interface quality, band offsets, back-contact properties, and optical absorption. This interdependence explains why improving only one parameter, such as absorber thickness, is often insufficient to achieve a major efficiency enhancement^{15–20}. In

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conventional Sb_2Se_3 thin-film solar cells, device performance is strongly affected by absorber orientation, buffer/absorber band alignment, back-contact quality, and defect-assisted recombination at internal interfaces²¹.

One promising strategy to overcome the intrinsic limitations of single-absorber Sb_2Se_3 devices is the introduction of a secondary absorber layer. A properly selected secondary absorber can broaden spectral utilization, improve carrier generation in selected wavelength regions, modify the internal electric-field distribution, and assist charge separation through favorable band alignment. In such a dual-absorber configuration, the second absorber is not merely an optical additive; it can also play an electronic role by altering recombination pathways, carrier-selective transport, and built-in potential. This concept is particularly attractive for Sb_2Se_3 solar cells because the main performance bottlenecks are strongly linked to carrier management rather than insufficient light absorption alone^{22–29}. CuGaSe_2 is a promising candidate for this purpose. As a chalcopyrite semiconductor, CuGaSe_2 exhibits a relatively wide bandgap of approximately 1.68 eV and strong absorption in the visible region, making it suitable for harvesting higher-energy photons. When integrated with a narrower-bandgap absorber such as Sb_2Se_3 , CuGaSe_2 can potentially contribute to complementary spectral absorption while also modifying the heterojunction energetics. In proposed cell, the CuGaSe_2 layer can act as an additional absorber positioned near the front junction region, where high-energy photon absorption and carrier separation are particularly critical. If the band alignment and defect density are properly controlled, this configuration may potentially enhance photovoltaic performance compared with the corresponding Sb_2Se_3 single-absorber reference device³⁰.

However, the introduction of an additional absorber layer also raises important physical questions. A secondary absorber may enhance photocurrent generation, but it may also introduce extra interfaces where recombination can occur. Therefore, the net performance improvement depends on the balance between additional optical absorption and possible recombination losses at the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ and $\text{CuGaSe}_2/\text{CdS}$ interfaces. For this reason, a rigorous device-level investigation is required before such an architecture can be considered physically meaningful. In particular, it is necessary to examine not only the current–voltage characteristics, but also the external quantum efficiency, generation and recombination profiles, capacitance–voltage behavior, activation energy, and impedance response. These analyses provide a deeper understanding of whether performance enhancement originates from improved light harvesting, better carrier separation, reduced recombination, or a combination of these mechanisms^{8,31–34}.

Numerical simulation is a powerful approach for studying such complex multilayer devices because it allows individual material and interface parameters to be varied systematically. SCAPS-1D, a one-dimensional solar cell capacitance simulator, has been extensively used for modeling thin-film heterojunction solar cells, including chalcogenide, *CdTe*, *CIGS*, kesterite, and emerging photovoltaic devices. The software solves the coupled Poisson and carrier-continuity equations and provides access to key photovoltaic characteristics such as J–V curves, quantum efficiency, band diagrams, generation–recombination profiles, capacitance–voltage response, and temperature-dependent behavior³⁵. Nevertheless, simulation-based studies must be carefully validated against experimental reference data, because unrealistic input parameters or physically inconsistent assumptions can lead to overestimated efficiencies. Therefore, a credible numerical study should first reproduce a reliable reference cell and then evaluate the proposed modification under comparable structural and physical conditions^{36,37}. In this work, a dual-absorber $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ thin-film solar cell is proposed and numerically investigated using SCAPS-1D. To isolate the effect of CuGaSe_2 , the comparison is performed under identical Sb_2Se_3 absorber thickness and transport-layer configuration, so that the observed performance changes can be directly attributed to the incorporation of the CuGaSe_2 secondary absorber. The numerical model is first validated using the photovoltaic characteristics of the reference Sb_2Se_3 solar cell, including J–V and EQE behavior. After validation, the influence of CuGaSe_2 on photovoltaic output parameters, optical absorption, spectral response, carrier generation, recombination loss, built-in potential, activation energy, and impedance response is systematically analyzed^{38–40}.

In this work, a CuGaSe_2 -assisted Sb_2Se_3 dual-absorber thin-film solar cell is proposed and numerically investigated using SCAPS-1D. The reference Sb_2Se_3 device is first calibrated against experimentally reported photovoltaic characteristics, including J–V and EQE behavior. After calibration, the effect of inserting CuGaSe_2 between Sb_2Se_3 and CdS is systematically examined in terms of photovoltaic output parameters, spectral response, carrier generation, recombination behavior, band alignment, built-in potential, activation energy, and impedance response. The aim is to clarify whether CuGaSe_2 can function not only as a secondary absorber but also as an interfacial energy-modulating layer for improving carrier separation and recombination management.

Device structure and simulation methodology

The numerical investigation was performed using the one-dimensional SCAPS simulator to evaluate the photovoltaic performance of Sb_2Se_3 -based thin-film solar cells with and without a CuGaSe_2 intermediate absorber layer. The simulated reference and proposed device architectures are schematically illustrated in Fig. 1b. The reference cell consists of the conventional stack: $\text{Mo}/\text{MoSe}_2/\text{Sb}_2\text{Se}_3/\text{CdS}/\text{ZnO}/\text{Al:ZnO}$, where Mo acts as the back contact, MoSe_2 is used as the hole-transport/passivation layer, Sb_2Se_3 serves as the main absorber, CdS is employed as the buffer layer, ZnO functions as the electron-transport layer, and Al-doped ZnO is used as the transparent window/contact layer.

In Fig. 1a CuGaSe_2 layer is inserted between the Sb_2Se_3 absorber and the CdS buffer layer, resulting in the following structure:

$\text{Mo}/\text{MoSe}_2/\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2/\text{CdS}/\text{ZnO}/\text{Al:ZnO}$. The thickness of Sb_2Se_3 was fixed at 2.6 μm , while the CuGaSe_2 thickness was optimized by varying it from 0.2 to 2.0 μm . Based on this optimization, a CuGaSe_2 thickness of 1.0 μm was selected for the proposed device because it provided the highest efficiency and the best compromise between additional photon absorption and recombination/transport losses.

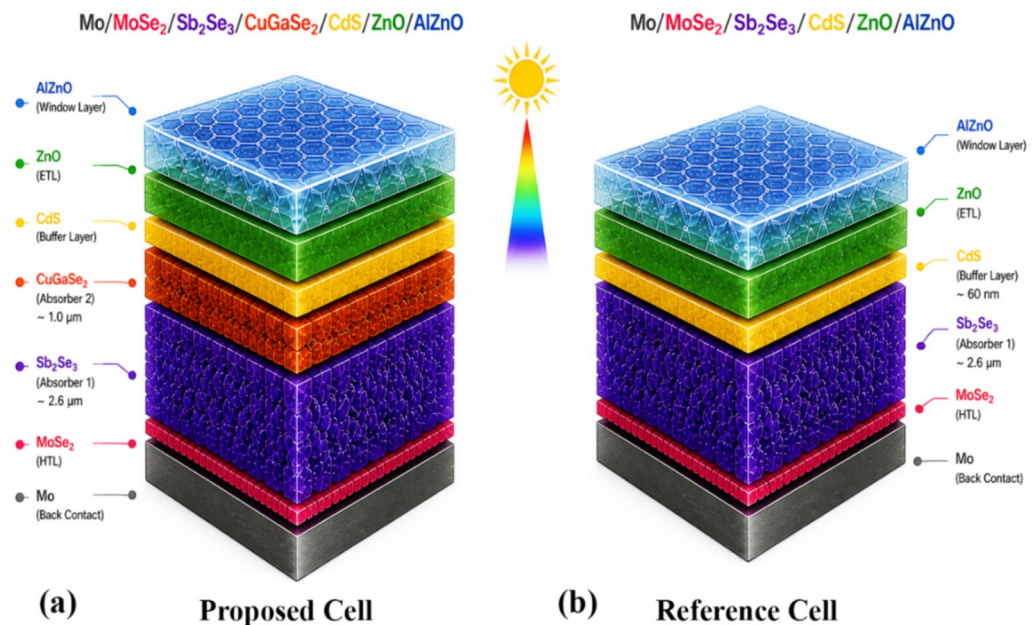


Fig. 1. Schematic representation of the simulated Sb_2Se_3 -based thin-film solar cells: (a) proposed device with the $\text{Mo}/\text{MoSe}_2/\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2/\text{CdS}/\text{ZnO}/\text{AlZnO}$ configuration and (b) reference device with the $\text{Mo}/\text{MoSe}_2/\text{Sb}_2\text{Se}_3/\text{CdS}/\text{ZnO}/\text{AlZnO}$ configuration. In the proposed structure, a $1.0\ \mu\text{m}$ CuGaSe_2 secondary absorber is inserted between the $2.6\ \mu\text{m}$ Sb_2Se_3 absorber and the $60\ \text{nm}$ CdS buffer layer to enhance short-/visible-wavelength photon utilization and modify the absorber/buffer interfacial energetics.

The CuGaSe_2 thickness of $1.0\ \mu\text{m}$ was selected as a physically reasonable representative value to evaluate the dual-absorber concept. This value was not intended to represent a global thickness optimum; rather, it provides a compromise between additional photon absorption and carrier-transport/recombination considerations. A thinner CuGaSe_2 layer would reduce the contribution of the secondary absorber to photogeneration, whereas an excessively thick CuGaSe_2 layer could increase the carrier-transport path and enhance recombination losses. Therefore, $1.0\ \mu\text{m}$ was used as a representative thickness for assessing the potential of the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer absorber architecture. A systematic optimization of the CuGaSe_2 thickness will be considered in future work.

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The CdS buffer layer thickness was kept at $60\ \text{nm}$ in both the reference and proposed structures. Therefore, the main structural modification in the proposed device is the incorporation of CuGaSe_2 as a secondary absorber layer. This design was considered to enhance photon harvesting, improve carrier generation, and modify the internal carrier-transport pathway without changing the front window and buffer-layer configuration. The physical operation of the devices was calculated by solving Poisson's equation and the electron and hole continuity equations under steady-state illumination. The drift–diffusion transport model was used to describe carrier motion across the multilayer structure. Recombination mechanisms, including Shockley–Read–Hall recombination, radiative recombination, and Auger recombination, were considered in the simulation framework.

The principal material parameters used for the SCAPS-1D simulation are summarized in Table 1.

The numerical calculations were carried out by solving the coupled Poisson and carrier-continuity equations under steady-state illumination. The electrostatic potential ψ was obtained from Poisson's equation:

$$\frac{d}{dx} \left(\varepsilon \frac{d\psi}{dx} \right) = -q \left(p - n + N_D^+ - N_A^- + \frac{\rho_t}{q} \right) \quad (1)$$

where ε is the dielectric permittivity, n and p are the electron and hole concentrations, N_D^+ and N_A^- are the ionized donor and acceptor densities, and ρ_t represents the charge associated with trap states. The electron and hole continuity equations were expressed as:

$$\frac{dJ_n}{dx} = q(R - G) \quad (2)$$

Parameters	Sb ₂ Se ₃	CuGaSe ₂	CdS	ZnO	ZnO:Al	MoSe ₂
Thickness (μm)	2.6	1	0.06	0.1	0.3	0.002
E_g (eV)	1.1	1.68	2.42	3.3	3.6	1.4
χ_e (eV)	4.16	4.3	4.45	4.5	4.5	4.32
ϵ_r	19	13.6	10	9	9	7.29
N_c (cm ⁻³)	1×10^{19}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	9×10^{18}
N_v (cm ⁻³)	1×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	9×10^{18}
$v_{th,e}$ (cm/s)	10^7	10^7	10^7	10^7	10^7	10^7
$v_{th,h}$ (cm/s)	10^7	10^7	10^7	10^7	10^7	10^7
μ_e (cm ² /Vs)	15	100	100	100	100	25
μ_h (cm ² /Vs)	5.1	25	25	25	25	100
Doping (cm ⁻³)	7×10^{13} (A)	1×10^{15} (A)	7.12×10^{17} (D)	6.77×10^{18} (D)	10^{20} (D)	5×10^{19} (A)

Table 1. Principal material parameters used in the SCAPS-1D simulation for the proposed and conventional Sb₂Se₃-based solar cells. The complete calibrated input dataset, including defect parameters, interface trap densities, recombination coefficients, optical absorption files, and contact work functions, is provided in Tables 2 and 3, and in the supplementary SCAPS definition files.^{17,33,41}

$$\frac{dJ_p}{dx} = q(G - R) \quad (3)$$

where G and R are the optical generation and total recombination rates, respectively. Carrier transport was described using the drift–diffusion model:

$$J_n = q\mu_n nE + qD_n \frac{dn}{dx} \quad (4)$$

$$J_p = q\mu_p pE - qD_p \frac{dp}{dx} \quad (5)$$

where μ_n and μ_p are the electron and hole mobilities, D_n and D_p are the diffusion coefficients, and E is the internal electric field. The total recombination rate was calculated by considering Shockley–Read–Hall, radiative, and Auger recombination:

$$R_{\text{tot}} = R_{\text{SRH}} + R_{\text{rad}} + R_{\text{Auger}} \quad (6)$$

The SRH recombination rate was given by:

$$R_{\text{SRH}} = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \quad (7)$$

while the radiative and Auger recombination terms were expressed as:

$$R_{\text{rad}} = B(np - n_i^2) \quad (8)$$

$$R_{\text{Auger}} = (C_n n + C_p p)(np - n_i^2) \quad (9)$$

where B is the radiative recombination coefficient and C_n and C_p are the electron and hole Auger coefficients. The optical generation rate was calculated using the wavelength-dependent absorption coefficient of each layer:

$$G(x) = \int \alpha(\lambda, x) \Phi(\lambda, x) d\lambda \quad (10)$$

where $\alpha(\lambda, x)$ is the absorption coefficient and $\Phi(\lambda, x)$ is the local photon flux inside the device. All simulations were performed under AM1.5G illumination at 300 K.

The optical generation profile was calculated from the wavelength-dependent absorption coefficients of the constituent layers. In particular, the absorption contribution of CuGaSe₂ was included in the proposed structure to evaluate its role in extending the photogeneration region and improving the short-circuit current density.

Before analyzing the proposed Sb₂Se₃/CuGaSe₂ bilayer absorber architecture, the numerical model was first calibrated against an experimentally reported Sb₂Se₃ solar cell in order to ensure the reliability of the simulation framework. The calibration procedure is presented in Fig. 2, where four independent photovoltaic characteristics were compared between the experimental device and the SCAPS-simulated reference cell. Figure 2a compares the wavelength-dependent integrated photocurrent density obtained from the experimental external quantum efficiency response and the corresponding simulated result. The close overlap between the experimental and

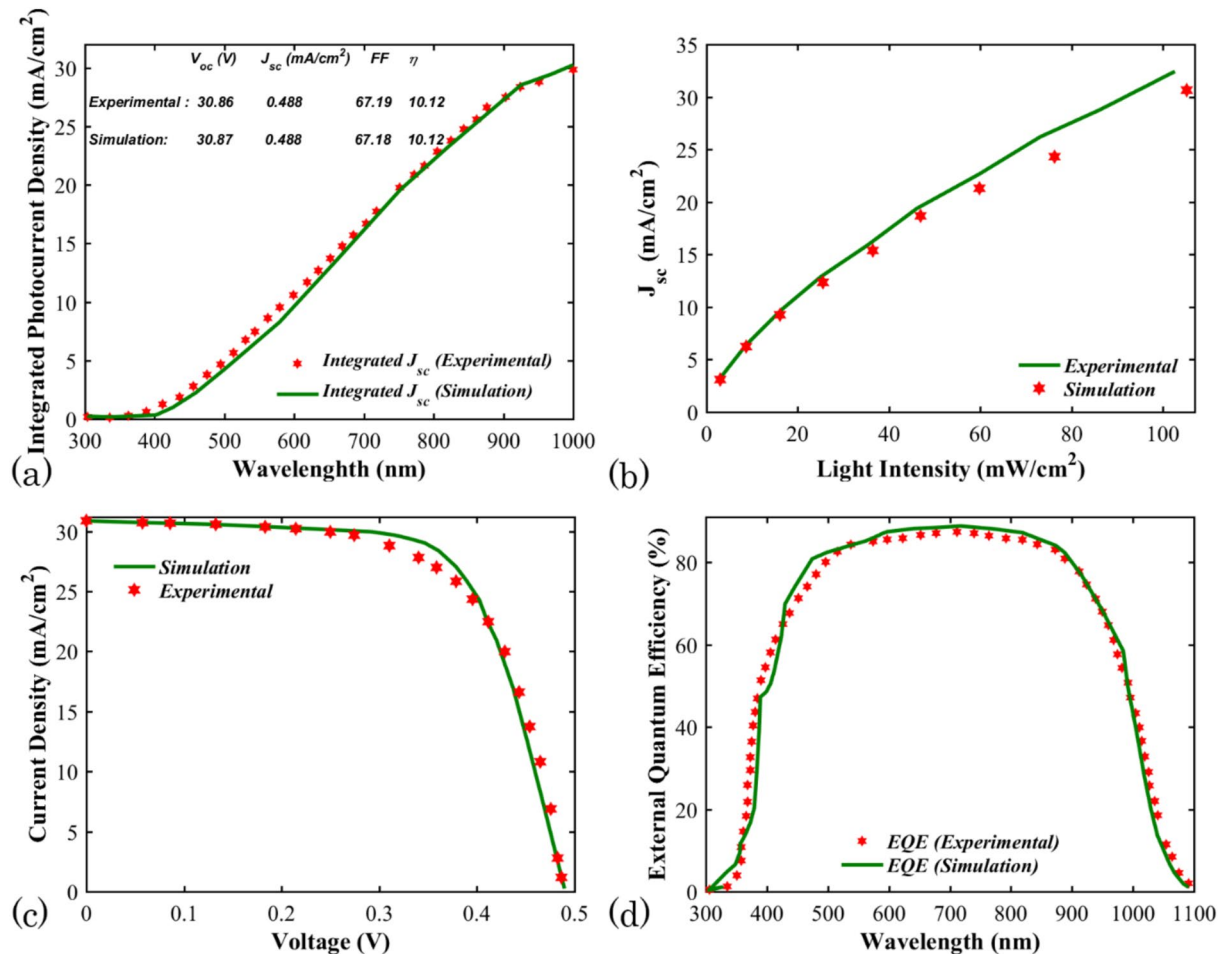


Fig. 2. Calibration of the SCAPS-1D simulation model using an experimentally reported Sb₂Se₃ solar cell³⁹: (a) integrated photocurrent density as a function of wavelength, (b) short-circuit current density under different light intensities, (c) current density–voltage characteristics, and (d) external quantum efficiency spectra. The calibrated simulation reproduces the experimental photovoltaic parameters with excellent agreement: $J_{sc} = 30.87 \text{ mA cm}^{-2}$, $V_{oc} = 0.488 \text{ V}$, $FF = 67.18\%$, and $\eta = 10.12\%$, confirming the reliability of the reference model for further device analysis.

simulated curves indicates that the optical absorption profile, spectral carrier generation, and wavelength-dependent photocurrent contribution were accurately reproduced in the simulation. This agreement is particularly important because the integrated photocurrent directly reflects the consistency between the optical input data, absorber thickness, and carrier collection efficiency used in the numerical model. Figure 2b, shows the variation of short-circuit current density as a function of incident light intensity. The simulated values follow the same increasing trend as the experimental data over the investigated illumination range, confirming that the model can correctly describe the light-dependent photocurrent generation behavior of the Sb₂Se₃ device. The agreement in this plot suggests that the selected material parameters and recombination settings provide a realistic description of carrier generation and collection under different illumination conditions.

The current density–voltage characteristics of the calibrated reference device are shown in Fig. 2c. The simulated J–V curve closely matches the experimental curve, especially in terms of short-circuit current density, open-circuit voltage, and the overall shape of the diode response. The experimental device exhibited $J_{sc} = 30.86 \text{ mA cm}^{-2}$, $V_{oc} = 0.488 \text{ V}$, $FF = 67.19\%$, and $\eta = 10.12\%$, while the SCAPS simulation yielded $J_{sc} = 30.87 \text{ mA cm}^{-2}$, $V_{oc} = 0.488 \text{ V}$, $FF = 67.18\%$, and $\eta = 10.12\%$. The negligible deviation between the experimental and simulated photovoltaic parameters confirms that the electrical properties of the device, including bulk defects, interface recombination, carrier transport, and contact behavior, were properly calibrated. Figure 2d, further validates the model by comparing the experimental and simulated external quantum efficiency spectra. The simulated EQE curve reproduces the main spectral features of the experimental response, including the sharp increase in the short-wavelength region, the broad high-response plateau in the visible range, and the gradual reduction near the long-wavelength absorption edge. This agreement confirms that the calibrated model can accurately describe wavelength-dependent absorption and carrier collection in the reference Sb₂Se₃ solar cell. Overall, the excellent agreement observed in Fig. 2a–d, demonstrates that the simulation model is sufficiently reliable for further device analysis. Therefore, the calibrated material parameters, defect densities,

Parameters	Sb ₂ Se ₃	CuGaSe ₂	CdS	ZnO	ZnO:Al	MoSe ₂
Bulk defect density, N_t (cm ⁻³)	10 ¹⁴	10 ¹⁴	10 ¹⁵	10 ¹⁵	10 ¹⁵	10 ¹⁴
Defect type	Neutral	Neutral	Neutral	Neutral	Neutral	Neutral
Energetic distribution	Single level	Single level	Single level	Single level	Single level	Single level
Trap energy level, E_t	$E_v+0.55$ eV	$E_v+0.84$ eV	$E_v+1.21$ eV	$E_v+1.65$ eV	$E_v+1.8$ eV	$E_v+0.7$ eV
Electron capture cross-section, σ_n (cm ²)	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵
Hole capture cross-section, σ_p (cm ²)	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵
Radiative recombination coefficient, B (cm ³ s ⁻¹)	10 ⁻¹⁰	10 ⁻¹⁰	10 ⁻¹⁰	10 ⁻¹⁰	10 ⁻¹⁰	10 ⁻¹⁰
Electron Auger coefficient, C_n (cm ⁶ s ⁻¹)	10 ⁻³⁰	10 ⁻³⁰	10 ⁻³⁰	10 ⁻³⁰	10 ⁻³⁰	10 ⁻³⁰
Hole Auger coefficient, C_p (cm ⁶ s ⁻¹)	10 ⁻³⁰	10 ⁻³⁰	10 ⁻³⁰	10 ⁻³⁰	10 ⁻³⁰	10 ⁻³⁰

Table 2. Additional bulk defect and recombination parameters used in the calibrated SCAPS-1D simulations.

Interface	Device	N_t (cm ⁻²)	Defect type	Energetic distribution	Energy level	σ_n (cm ²)	σ_p (cm ⁻²)
Sb ₂ Se ₃ /CdS	Reference cell	10 ¹²	Neutral	Single level	Mid-gap	10 ⁻¹⁵	10 ⁻¹⁵
Sb ₂ Se ₃ /CuGaSe ₂	Proposed cell	10 ¹²	Neutral	Single level	Mid-gap	10 ⁻¹⁵	10 ⁻¹⁵
CuGaSe ₂ /CdS	Proposed cell	10 ¹²	Neutral	Single level	Mid-gap	10 ⁻¹⁵	10 ⁻¹⁵

Table 3. Interface defect parameters used in the calibrated reference and proposed SCAPS-1D simulations.

interface properties, and optical inputs were used as the basis for investigating the proposed CuGaSe₂-assisted Sb₂Se₃ solar-cell architecture.

In addition to the principal layer parameters listed in Table 1, the calibrated SCAPS-1D model also requires bulk defect, recombination, interface-defect, and contact parameters. These additional input parameters are summarized in Tables 2 and 3 to improve the reproducibility of the numerical results and to clarify the origin of the difference between the calibrated simulation and simulations performed using only the basic layer parameters.

It should be emphasized that Table 1 lists the principal material parameters, whereas Tables 2 and 3 provide the additional defect, recombination, and interface parameters required to reproduce the calibrated SCAPS-1D results. Therefore, using only the basic parameters in Table 1 together with default or idealized SCAPS settings may lead to different photovoltaic outputs, particularly an overestimated J_{sc} and fill factor. In the present work, the calibrated reference-cell parameters were obtained using the complete input dataset, including the wavelength-dependent absorption files, calibrated bulk and interface defect states, recombination coefficients, and contact properties.

The physical and electronic parameters used for the SCAPS-1D simulation are summarized in Table 1. These parameters define the optical absorption, carrier transport, electrostatic potential distribution, and recombination behavior of each layer in the simulated solar-cell structures. The layer thickness determines the optical absorption volume and carrier-collection length, while the band gap (E_g) and electron affinity (χ_e) govern the band alignment at the heterointerfaces. In particular, the electron-affinity difference between adjacent layers plays a critical role in determining the conduction-band offset, which strongly influences electron extraction, interface recombination, and carrier-blocking behavior. The relative dielectric constant (ϵ_r), effective density of states in the conduction and valence bands (N_c and N_v), carrier thermal velocities ($v_{th,e}$ and $v_{th,h}$), mobilities (μ_e and μ_h), and doping concentration were selected to represent physically realistic transport and recombination conditions in each material layer. These parameters directly affect the built-in electric field, depletion width, carrier diffusion length, and recombination probability within the absorber and transport layers. Therefore, careful selection of these values is essential for obtaining reliable numerical results.

The relatively high donor concentrations used for ZnO and Al:ZnO reflect their roles as electron-transport and transparent-conducting oxide layers rather than absorber layers. Such high carrier densities are experimentally realistic for doped ZnO-based films. Experimental studies have reported carrier concentrations in the range of 10¹⁸–10²⁰ cm⁻³ for highly doped ZnO and Al-doped ZnO thin films^{42–44}. Therefore, the donor concentrations used for ZnO and Al:ZnO are consistent with highly conductive ZnO-based transport/contact layers. The high acceptor concentration assigned to the ultrathin MoSe₂ layer should be interpreted as an effective parameter representing a highly conductive hole-selective back-contact/passivation layer rather than a thick bulk absorber. This treatment is commonly adopted in numerical modeling to describe strongly conductive interfacial layers that reduce back-contact barriers and facilitate hole extraction.

It should be emphasized that Table 1 summarizes the principal material parameters of the semiconductor layers. However, reproducing the calibrated reference-cell result requires the complete SCAPS input dataset, including wavelength-dependent absorption files, bulk defect parameters, interface trap densities, recombination coefficients, and contact work functions. If only the basic parameters listed in Table 1 are used together with idealized or default optical, defect, interface, and contact settings, SCAPS may overestimate the photocurrent and fill factor. In the present work, the reference device was calibrated against the experimentally reported

Sb_2Se_3 solar cell by matching the J–V curve, EQE spectrum, integrated photocurrent density, and light-intensity-dependent J_{sc} . Therefore, the calibrated photovoltaic parameters are obtained only when the complete SCAPS definition file is used. To improve reproducibility, the full SCAPS definition files for both the calibrated reference cell and the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ dual-absorber cell are provided as supplementary files.

The Mo back contact was defined using a work function of $\Phi_{Mo} = 5.0$ eV. This contact, together with the ultrathin MoSe_2 interlayer, was used to form a hole-selective back-contact configuration and to reduce the back-interface transport barrier.

For a fair comparison between the reference and proposed devices, the same material parameters were used for the common layers, including MoSe_2 , Sb_2Se_3 , CdS , ZnO , and Al:ZnO . The main structural modification in the proposed device is the insertion of the CuGaSe_2 absorber layer between Sb_2Se_3 and CdS . This approach allows the effect of the secondary absorber layer on optical generation, carrier separation, recombination suppression, and overall photovoltaic performance to be evaluated systematically. The calibrated model was then used as the baseline for further device engineering. After achieving agreement between the simulated and experimental reference cell, the CuGaSe_2 layer was introduced into the absorber stack while keeping the other major layers unchanged. This approach ensures that the observed changes in device performance originate mainly from the CuGaSe_2 incorporation rather than from arbitrary changes in the simulation environment. The photovoltaic response of both devices was evaluated under standard AM1.5G illumination at room temperature. The main extracted parameters were open-circuit voltage, short-circuit current density, fill factor, and power conversion efficiency. In addition, generation-rate profiles, recombination-rate distributions, external quantum efficiency spectra, and current–voltage characteristics were analyzed to clarify the physical origin of the performance variation.

The purpose of inserting CuGaSe_2 was not only to increase the optical absorption volume but also to create a more favorable absorber configuration for carrier generation and extraction. Since CuGaSe_2 is a direct-bandgap chalcopyrite semiconductor with strong optical absorption, its incorporation can contribute to additional photon absorption in the visible and near-infrared spectral regions. Moreover, the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer absorber structure may influence the internal electric field and carrier distribution, thereby affecting the balance between photogeneration and recombination. Therefore, the proposed structure was evaluated not only from the viewpoint of efficiency enhancement, but also in terms of its physical consistency through generation, recombination, and EQE analyses.

Results and discussion

Optical absorption characteristics of the constituent layers

The optical response of each layer plays a decisive role in determining the carrier-generation capability of thin-film photovoltaic devices. Therefore, before evaluating the complete device performance, the wavelength-dependent absorption coefficients of the main functional layers were analyzed, as shown in Fig. 3. The absorption spectra of Sb_2Se_3 , CdS , ZnO , Al:ZnO , and CuGaSe_2 were introduced into the simulation to ensure that the optical generation profile was calculated using realistic wavelength-dependent material data. As shown in Fig. 3a, Sb_2Se_3 exhibits a strong absorption coefficient in the visible region, confirming its suitability as the primary absorber layer. Its absorption remains high over a broad spectral range and gradually decreases at longer

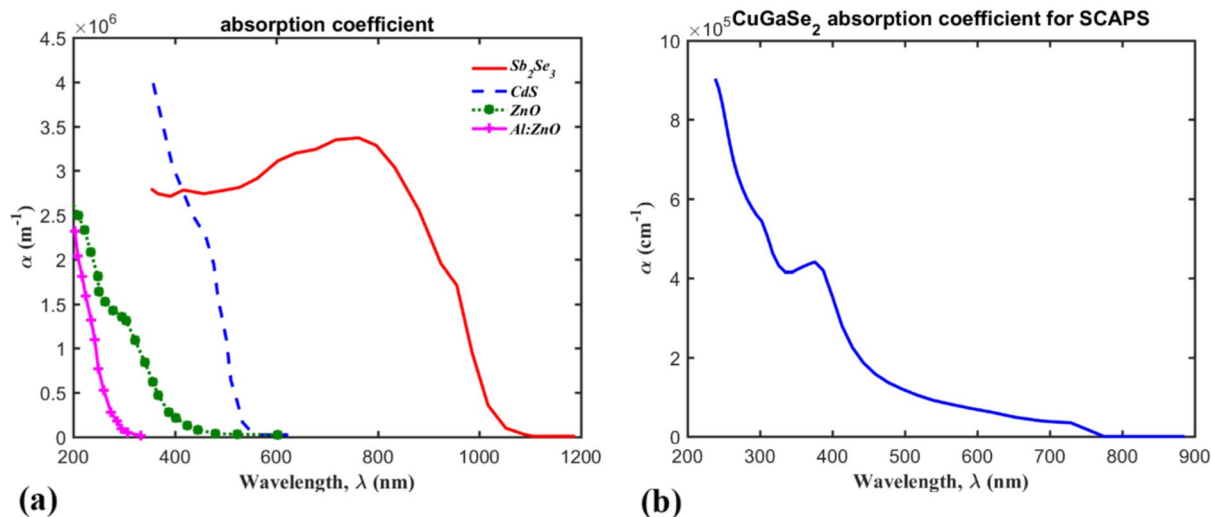


Fig. 3. Wavelength-dependent absorption coefficients used in the SCAPS-1D simulation: (a) absorption spectra of Sb_2Se_3 , CdS , ZnO , and Al:ZnO layers, and (b) absorption coefficient of CuGaSe_2 introduced as the secondary absorber layer²⁹. Sb_2Se_3 , with $E_g = 1.10$ eV, provides broadband absorption extending toward the near-infrared region, whereas CuGaSe_2 , with $E_g = 1.68$ eV, mainly contributes to short- and visible-wavelength photon absorption. The window and buffer layers show comparatively limited absorption in the visible/near-infrared range, reducing parasitic optical losses³⁰.

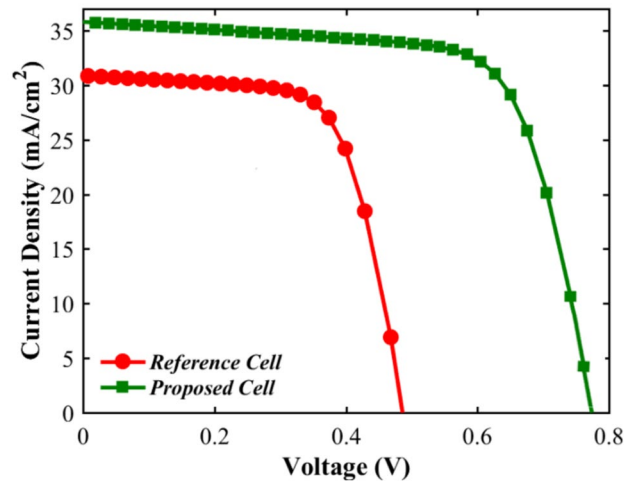


Fig. 4. Current density–voltage characteristics of the reference and proposed Sb_2Se_3 -based solar cells under AM1.5G illumination. The proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ dual-absorber cell improves J_{sc} from 30.87 to 35.80 mA cm^{-2} , V_{oc} from 0.48 to 0.77 V, FF from 67.18 to 70.28%, and efficiency from 10.12 to 19.50%. The dominant improvement is associated with the substantial V_{oc} enhancement and recombination suppression, while the J_{sc} increase provides an additional photocurrent contribution.

Device	V_{oc} (V)	J_{sc} (mA.cm^{-2})	FF (%)	η (%)
Reference cell	0.48	30.87	67.18	10.12
Proposed cell	0.77	35.80	70.28	19.50
Improvement	+ 0.29 V	+ 4.93 mA.cm^{-2}	+ 3.10%	+ 9.38% absolute

Table 4. Photovoltaic parameters extracted from the J–V characteristics of the reference and proposed solar cells under AM1.5G illumination.

wavelengths. In contrast, CdS, ZnO, and Al:ZnO mainly absorb in the shorter-wavelength region, while their absorption becomes negligible in the visible and near-infrared range. This behavior is favorable because these layers are intended to function as buffer, electron-transport, and window layers rather than active absorbers. The absorption coefficient of CuGaSe_2 , shown separately in Fig. 3b, confirms its strong optical activity in the visible region. CuGaSe_2 exhibits additional optical absorption in this spectral range, which contributes to enhanced photon harvesting and increased photogeneration within the absorber stack. Although its absorption coefficient decreases toward longer wavelengths, it remains significant over a broad portion of the solar spectrum. Therefore, its incorporation into the absorber stack can increase the total photogenerated carrier density, particularly in wavelength regions where Sb_2Se_3 exhibits weaker absorption. Overall, the optical analysis supports the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer configuration as a promising strategy for improved light harvesting.

Photovoltaic performance of the reference and proposed cells

The current density–voltage characteristics of the reference and proposed Sb_2Se_3 -based solar cells under standard AM1.5G illumination are shown in Fig. 4, and the corresponding photovoltaic parameters are summarized in Table 4. The reference device, based on the $\text{Sb}_2\text{Se}_3/\text{CdS}$ configuration, exhibits a power conversion efficiency of 10.12%, with a short-circuit current density of 30.87 mA cm^{-2} , an open-circuit voltage of 0.48 V, and a fill factor of 67.18%. After introducing the CuGaSe_2 layer into the absorber architecture, the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ -based device shows a remarkable enhancement in overall photovoltaic performance, reaching a J_{sc} of 35.80 mA cm^{-2} , a V_{oc} of 0.77 V, a fill factor of 70.28%, and a power conversion efficiency of 19.50%. The performance parameters listed in Table 4 clearly indicate that the improvement in the proposed device is not limited to a single photovoltaic parameter, but results from the simultaneous enhancement of J_{sc} , V_{oc} , and FF. The increase in J_{sc} from 30.87 to 35.80 mA cm^{-2} suggests that the incorporation of CuGaSe_2 improves photon harvesting and carrier generation within the device. This behavior can be attributed to the additional optical absorption contribution of the CuGaSe_2 layer, which acts as a secondary absorber and enables more effective utilization of incident photons. Therefore, the enhanced photocurrent density confirms that the CuGaSe_2 layer actively contributes to charge generation rather than behaving as an optically inactive interlayer. A more significant improvement is observed in the open-circuit voltage, which increases from 0.48 in the reference cell to 0.77 V in the proposed structure. This substantial V_{oc} enhancement suggests that the CuGaSe_2 layer plays an important role in modifying the internal electrical behavior of the device. In particular, the improved voltage output can be associated with more favorable band alignment, enhanced carrier separation, improved junction quality, and reduced recombination-related voltage losses. Since V_{oc} is strongly governed by

recombination mechanisms and quasi-Fermi level splitting, the higher V_{oc} obtained for the proposed device indicates that the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ absorber configuration provides a more efficient pathway for suppressing non-radiative recombination and improving charge selectivity.

The fill factor also increases from 67.18 to 70.28%, confirming that the insertion of CuGaSe_2 does not introduce severe transport barriers or detrimental resistive losses. Since FF is sensitive to carrier transport, series resistance, shunt resistance, junction quality, and recombination losses, its improvement indicates more efficient charge extraction in the proposed device. As a result, the combined enhancement in J_{sc} , V_{oc} , and FF leads to a substantial increase in power conversion efficiency from 10.12 to 19.50%. Overall, the results presented in Fig. 4, and Table 4, demonstrate that the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ absorber design provides a balanced optical and electrical improvement, making it a promising architecture for high-performance Sb_2Se_3 -based thin-film solar cells.

Role of the CuGaSe_2 layer in absorber engineering

To isolate the physical contribution of the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ dual-absorber configuration, the current density–voltage characteristics of the bilayer device were compared with two single-absorber counterparts, as shown in Fig. 5. Figure 5a, compares the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ absorber stack with a single CuGaSe_2 absorber, while Fig. 5b, compares the same bilayer configuration with a single Sb_2Se_3 absorber of identical Sb_2Se_3 thickness. This comparison is essential because it distinguishes the true dual-absorber effect from a simple thickness-induced enhancement. As shown in Fig. 5a, the single CuGaSe_2 absorber exhibits a relatively high open-circuit voltage but a considerably limited current density. This behavior is consistent with its wider bandgap, which enhances quasi-Fermi-level splitting, while its reduced absorption in the long-wavelength region limits photocurrent generation.

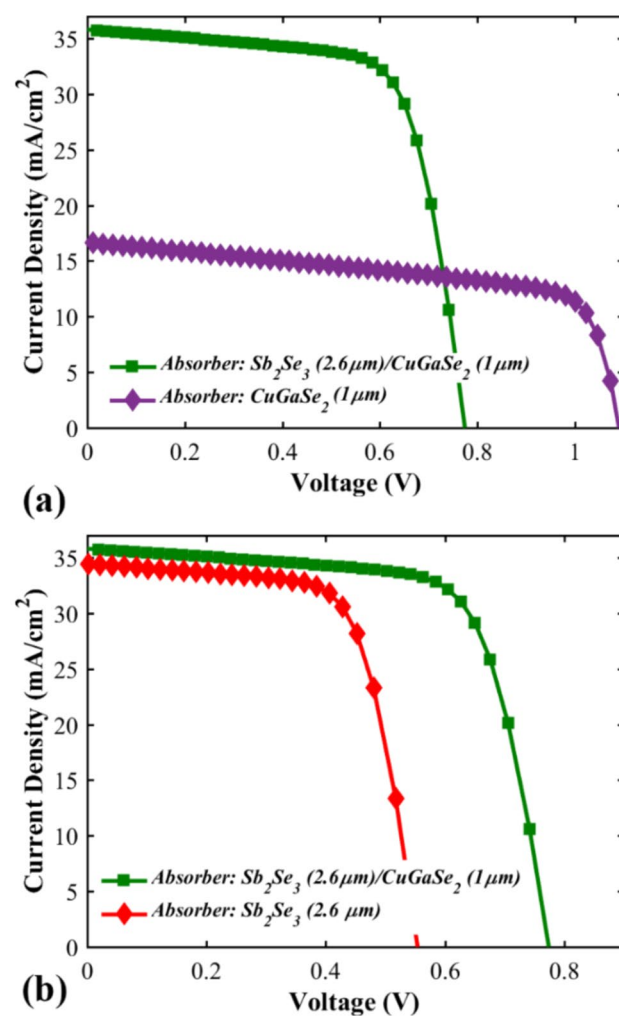


Fig. 5. Effect of absorber configuration on device performance: (a) comparison between the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer absorber and a CuGaSe_2 -only absorber, and (b) comparison between the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer absorber and a Sb_2Se_3 -only absorber. The bilayer device maintains the broadband photocurrent contribution of Sb_2Se_3 while gaining additional voltage enhancement from CuGaSe_2 -assisted interfacial energy modulation. The results confirm that the performance improvement is not a simple absorber-thickness effect but arises from the combined optical and electronic roles of the dual-absorber stack.

In contrast, the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer device exhibits a higher current density, reaching approximately 35–36 mA cm^{-2} , while maintaining a practically useful voltage level. This suggests that Sb_2Se_3 plays a dominant role in extending the spectral absorption range and enhancing photogenerated current, whereas CuGaSe_2 primarily contributes to improved junction properties and enhanced voltage output through favorable interfacial band alignment. In this context, CuGaSe_2 can be regarded as a multifunctional layer that simultaneously supports photon absorption and modulates interfacial energy levels, thereby facilitating improved carrier separation and reduced recombination losses.

The current generation in a bilayer absorber can be described by the wavelength-dependent absorbed photon flux. For a front CuGaSe_2 layer followed by Sb_2Se_3 , the short-circuit current density can be approximated as⁴⁵:

$$J_{sc} = q \int \Phi_{AM1.5G}(\lambda) \left[\eta_{CGS}(\lambda) (1 - e^{-\alpha_{CGS}(\lambda)t_{CGS}}) + \eta_{Sb}(\lambda) e^{-\alpha_{CGS}(\lambda)t_{CGS}} (1 - e^{-\alpha_{Sb}(\lambda)t_{Sb}}) \right] d\lambda \quad (11)$$

where q is the elementary charge, $\Phi_{AM1.5G}(\lambda)$ is the incident solar photon flux, α_{CGS} and α_{Sb} are the absorption coefficients of CuGaSe_2 and Sb_2Se_3 , t_{CGS} and t_{Sb} are their thicknesses, and η_{CGS} and η_{Sb} represent the corresponding carrier-collection efficiencies. This expression shows that the total photocurrent is not merely the sum of two independent absorbers. Instead, it depends on optical filtering by the upper absorber, residual photon absorption in the lower absorber, and the collection probability of carriers generated in each region. Therefore, the superior current density of the bilayer device in Fig. 5a, confirms that the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ stack provides a more complete utilization of the incident spectrum than the CuGaSe_2 -only structure. Figure 5b, provides an even more important comparison because the Sb_2Se_3 thickness is kept fixed while CuGaSe_2 is introduced as an additional absorber layer. The single Sb_2Se_3 device already shows a high short-circuit current density because Sb_2Se_3 can absorb a broad portion of the visible and near-infrared spectrum. However, its voltage is considerably lower, indicating stronger recombination losses and a larger voltage deficit. After introducing CuGaSe_2 , the current density is slightly improved, but the most pronounced enhancement appears in the voltage and fill-factor region. The bilayer device exhibits a clear rightward shift of the J-V curve, demonstrating that CuGaSe_2 does not only act as an optical absorber but also modifies the internal electrostatic and recombination behavior of the device. This improvement can be interpreted through the diode equation²³:

$$J(V) = J_{ph} - J_0 \left[\exp \left(\frac{qV}{nk_B T} \right) - 1 \right] \quad (12)$$

where J_{ph} is the photogenerated current density, J_0 is the reverse saturation current density, n is the ideality factor, k_B is the Boltzmann constant, and T is temperature. Under open-circuit conditions, $J(V_{oc}) = 0$, giving:

$$V_{oc} = \frac{nk_B T}{q} \ln \left(\frac{J_{ph}}{J_0} + 1 \right) \quad (13)$$

Accordingly, the increase in V_{oc} observed in Fig. 5b, cannot be explained only by the moderate increase in photocurrent. Since V_{oc} depends logarithmically on J_{ph} , a small increase in current would produce only a limited voltage gain. The substantial rightward shift of the bilayer J-V curve therefore implies a reduction in J_0 , which is directly associated with suppressed recombination, improved band alignment, and enhanced built-in electric field across the absorber/buffer region.

The voltage enhancement can be expressed more explicitly as:

$$\Delta V_{oc} = \frac{nk_B T}{q} \ln \left[\frac{J_{ph,DA}}{J_{ph,Sb}} \frac{J_{0,Sb}}{J_{0,DA}} \right] \quad (14)$$

where DA denotes the dual-absorber device and Sb denotes the single Sb_2Se_3 absorber. Since the current enhancement in Fig. 5b, is moderate, the dominant term responsible for the observed voltage improvement must be the reduction of $J_{0,DA}$. This means that the CuGaSe_2 layer contributes electronically by reducing recombination-driven dark current, rather than functioning only as an additional optical absorber. The fill factor improvement in the dual-absorber device further supports this interpretation. In practical solar cells, the fill factor is highly sensitive to recombination, series resistance, shunt leakage, and carrier-transport barriers. The sharper rectangularity of the green J-V curve compared with the single Sb_2Se_3 curve indicates more efficient carrier extraction and lower non-radiative loss. Therefore, the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ design provides a simultaneous enhancement in J_{sc} , V_{oc} , and FF, which is the key signature of a successful dual-absorber architecture.

Overall, Fig. 5, demonstrates that the performance enhancement of the proposed cell originates from a synergistic absorber design. The Sb_2Se_3 layer mainly strengthens broadband photon harvesting and photocurrent generation, while the CuGaSe_2 layer improves voltage formation, carrier separation, and recombination control. Therefore, the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer absorber should not be viewed as a simple thickness extension, but rather as a functional absorber-engineering strategy that combines optical current enhancement with electronic loss suppression.

This interpretation is further supported by the energy band diagrams shown in Fig. 6, where the insertion of CuGaSe_2 modifies the absorber/buffer band profile and provides a more favorable energetic pathway for carrier separation and transport.

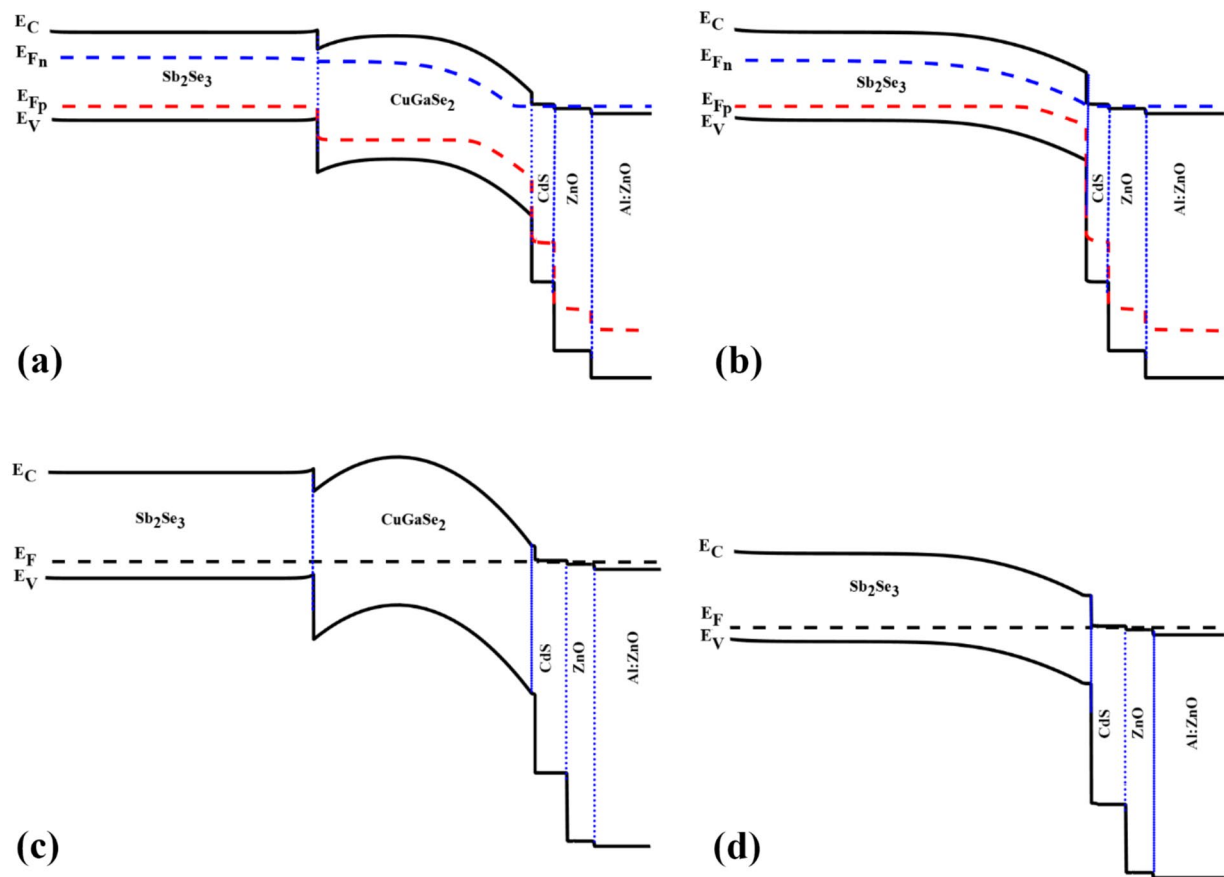


Fig. 6. Energy band diagrams of the proposed and reference Sb_2Se_3 -based solar cells under illumination and equilibrium conditions: (a) proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ device under AM1.5G illumination, (b) reference Sb_2Se_3 device under AM1.5G illumination, (c) proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ device under equilibrium, and (d) reference Sb_2Se_3 device under equilibrium. The diagrams show the conduction band minimum (E_C), valence band maximum (E_V), equilibrium Fermi level (E_F), and electron/hole quasi-Fermi levels (E_{Fn} and E_{Fp}). The calculated band offsets are $\Delta E_C = -0.14$ eV and $\Delta E_V = -0.72$ eV at the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ interface, and $\Delta E_C = -0.15$ eV and $\Delta E_V = -0.89$ eV at the $\text{CuGaSe}_2/\text{CdS}$ interface, supporting electron extraction toward CdS/ZnO while suppressing hole leakage and interfacial recombination.

CuGaSe ₂ thickness (μ m)	V _{oc} (V)	J _{sc} (mA cm ⁻²)	FF (%)	η (%)
0.0	0.488	30.87	67.18	10.12
0.2	0.620	32.40	68.20	13.70
0.4	0.690	33.70	69.00	16.04
0.6	0.735	34.60	69.70	17.73
0.8	0.763	35.40	70.10	18.93
1.0	0.775	35.80	70.28	19.50
1.2	0.774	35.85	69.65	19.33
1.5	0.770	35.75	68.90	18.97
2.0	0.762	35.40	67.80	18.29

Table 5. Effect of CuGaSe_2 thickness on the photovoltaic parameters of the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ dual-absorber solar cell.

Optimization of the CuGaSe_2 absorber thickness

Since the CuGaSe_2 layer plays a dual role as a secondary absorber and an interfacial energy-modulating layer, its thickness is an important design parameter. Therefore, the influence of CuGaSe_2 thickness on the photovoltaic performance of the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ device was systematically investigated. In this analysis, the CuGaSe_2 thickness was varied from 0.2 to 2.0 μ m, while all other material, defect, interface, and contact parameters were kept unchanged. The extracted photovoltaic parameters are summarized in Table 5.

As shown in Table 5, increasing the CuGaSe₂ thickness initially improves the photovoltaic performance. When the CuGaSe₂ thickness increases from 0.2 to 1.0 μm, the efficiency increases from 13.70 to 19.50%. This improvement is accompanied by an increase in J_{sc} from 32.40 to 35.80 mA cm⁻² and an increase in V_{oc} from 0.620 to 0.775 V. The enhancement in J_{sc} can be attributed to the increased absorption of short- and visible-wavelength photons by the CuGaSe₂ layer, while the improvement in V_{oc} is associated with more favorable absorber/buffer energetics and reduced recombination losses.

However, further increasing the CuGaSe₂ thickness beyond 1.0 μm does not lead to additional performance enhancement. At 1.2 μm, the efficiency slightly decreases to 19.33%, and it further decreases to 18.97% and 18.29% at 1.5 and 2.0 μm, respectively. This behavior indicates that excessively thick CuGaSe₂ does not provide a proportional optical benefit. Instead, it can increase the carrier-transport path and enhance recombination probability before carrier collection. In addition, because CuGaSe₂ has a wider bandgap than Sb₂Se₃, its optical contribution becomes limited once most above-bandgap photons have already been absorbed.

Therefore, the optimum CuGaSe₂ thickness is approximately 1.0 μm under the calibrated simulation conditions. This value provides the best compromise between additional photon absorption, carrier extraction, and recombination suppression. Accordingly, the 1.0 μm CuGaSe₂ thickness used in the proposed device is not arbitrary, but corresponds to the optimum thickness obtained from the systematic SCAPS-1D thickness optimization.

Layer-by-layer contribution analysis

To further clarify the individual contribution of each functional layer, a layer-by-layer control-device analysis was performed by comparing four device configurations under identical simulation conditions. The investigated structures were CdS/Sb₂Se₃, CdS/Sb₂Se₃/MoSe₂, CdS/CuGaSe₂/Sb₂Se₃, and CdS/CuGaSe₂/Sb₂Se₃/MoSe₂. This comparison allows the role of the CuGaSe₂ secondary absorber and the MoSe₂ back-contact/passivation layer to be separated more clearly. The extracted photovoltaic parameters are summarized in Table 6.

As shown in Table 6, the CdS/Sb₂Se₃ configuration without MoSe₂ exhibits the lowest performance, mainly because of less favorable back-contact selectivity and stronger back-interface recombination. After inserting the ultrathin MoSe₂ layer, the device performance improves, with V_{oc}, FF, and efficiency increasing. This confirms that MoSe₂ improves the back-contact region by facilitating hole extraction and reducing recombination losses at the rear interface. The improvement is more pronounced in voltage and fill factor than in current density, indicating that MoSe₂ primarily plays an electronic/passivation role rather than an optical role.

The introduction of CuGaSe₂ into the absorber stack produces a stronger improvement in the photovoltaic response. The CdS/CuGaSe₂/Sb₂Se₃ configuration exhibits a higher V_{oc} and J_{sc} than the single-absorber Sb₂Se₃ device, confirming that CuGaSe₂ contributes to both photon utilization and junction-quality improvement. However, the main performance gain remains associated with voltage enhancement and recombination suppression rather than with a purely current-driven effect. This is consistent with the comparative EQE analysis, which shows that CuGaSe₂ contributes mainly in the short- and visible-wavelength range, whereas Sb₂Se₃ remains the dominant absorber for long-wavelength and near-infrared photocurrent generation.

The highest efficiency is obtained for the complete CdS/CuGaSe₂/Sb₂Se₃/MoSe₂ configuration, corresponding to the proposed device. This result demonstrates that the improved device performance arises from the combined action of the CuGaSe₂ and MoSe₂ layers. CuGaSe₂ improves the front absorber/buffer energetics, enhances built-in potential, and suppresses recombination near the main junction, while MoSe₂ improves back-contact selectivity and hole extraction. Therefore, the proposed architecture should be regarded as a combined dual-absorber and interface-engineered structure rather than as a simple absorber-thickness extension.

The influence of the front-window layers was also considered. In the present comparison, ZnO and Al:ZnO were kept unchanged in all main device configurations; therefore, they do not account for the relative performance enhancement observed after CuGaSe₂ insertion. Nevertheless, these layers remain important for practical device operation. ZnO acts as an electron-transport/window layer, while Al:ZnO functions as the transparent conducting front contact. Their high bandgaps and optical transparency help reduce parasitic absorption in the visible and near-infrared regions, although some short-wavelength optical loss may still occur. If the front-window layers are excluded or replaced by an ideal transparent contact in SCAPS, the calculated J_{sc} may change slightly because of reduced parasitic absorption. However, such an idealized structure does not fully represent a practical device, because Al:ZnO is required to provide lateral conductivity and front-contact functionality. Therefore, the ZnO/Al:ZnO stack was retained as a physically realistic front-window/contact configuration. The dominant improvement in the proposed device is mainly attributed to the Sb₂Se₃/CuGaSe₂/MoSe₂ absorber/contact architecture rather than to changes in the front-window layers.

Device configuration	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	η (%)
CdS/Sb ₂ Se ₃	0.430	29.96	62.10	8.00
CdS/Sb ₂ Se ₃ /MoSe ₂	0.488	30.87	67.18	10.12
CdS/CuGaSe ₂ /Sb ₂ Se ₃	0.716	35.12	65.50	16.46
CdS/CuGaSe ₂ /Sb ₂ Se ₃ /MoSe ₂	0.775	35.80	70.28	19.50

Table 6. Layer-by-layer comparison of photovoltaic parameters for different device configurations under identical SCAPS-1D simulation conditions.

Accordingly, modification of ZnO or Al:ZnO may be useful for further optical optimization, but it does not change the central conclusion that CuGaSe₂ and MoSe₂ are the primary layers responsible for the enhanced voltage formation, recombination suppression, and carrier collection in the proposed architecture.

Energy band alignment and quasi-fermi level analysis

To provide direct visual evidence for the role of interfacial energetics in the proposed device, the energy band diagrams of the reference and CuGaSe₂-assisted solar cells were analyzed under both equilibrium and AM1.5G illumination conditions, as shown in Fig. 6. The diagrams include the conduction band minimum (*E_C*), valence band maximum (*E_V*), equilibrium Fermi level (*E_F*), and the electron and hole quasi-Fermi levels (*E_{F_n}* and *E_{F_p}*) under illumination. Since the photovoltaic response of multilayer heterojunction solar cells is strongly governed by interfacial band offsets, band bending, and quasi-Fermi level splitting, this analysis provides direct physical evidence for the energetic effect of inserting CuGaSe₂ into the Sb₂Se₃-based absorber stack.

To quantify the interfacial band alignment, the conduction-band offset (CBO) and valence-band offset (VBO) at the Sb₂Se₃/CuGaSe₂ and CuGaSe₂/CdS interfaces were calculated using the electron-affinity rule. The conduction-band minimum and valence-band maximum of each semiconductor were estimated with respect to the vacuum level as

$E_C = -\chi$ (15)

$E_V = -(\chi + E_g)$ (16)

where χ is the electron affinity and E_g is the optical bandgap. For an interface between layer A and layer B, the band offsets were defined as

$\Delta E_C = E_{C,B} - E_{C,A} = \chi_A - \chi_B$ (17)

$\Delta E_V = E_{V,B} - E_{V,A} = (\chi_A + E_{g,A}) - (\chi_B + E_{g,B})$ (18)

Using the material parameters listed in Table 1a, the calculated band-edge positions and corresponding interface offsets are summarized in Table 7.

As shown in Table 7, the Sb₂Se₃/CuGaSe₂ interface exhibits a small negative conduction-band offset of −0.14 eV. This indicates that the conduction band of CuGaSe₂ lies slightly below that of Sb₂Se₃, forming a mild cliff-like alignment for electron transport from Sb₂Se₃ toward the front junction. Such a small conduction-band step can facilitate electron transfer without producing a large electron-blocking spike. At the same interface, the calculated valence-band offset is −0.72 eV, meaning that the valence band of CuGaSe₂ is located significantly deeper than that of Sb₂Se₃. This offset provides an energetic barrier against hole transport toward the front side and therefore improves carrier selectivity.

At the CuGaSe₂/CdS interface, the calculated CBO is −0.15 eV, while the VBO is −0.89 eV. The small negative CBO indicates that electrons can be transferred from CuGaSe₂ into CdS without a severe transport barrier. Meanwhile, the large VBO strongly blocks holes from reaching the CdS buffer layer, thereby reducing the probability of hole accumulation and interface recombination near the front junction. Therefore, the Sb₂Se₃/CuGaSe₂/CdS stack provides a cascade-like conduction-band pathway for electron extraction together with strong valence-band blocking for holes.

It should be noted that a highly negative CBO can enhance interface recombination in heterojunction solar cells. However, the CBO values calculated here are relatively small, approximately −0.14 to −0.15 eV, and therefore do not represent a severe cliff. Instead, they provide a moderate downhill pathway for electron collection. This interpretation is consistent with the increased built-in potential, enhanced quasi-Fermi level splitting, higher recombination resistance, and reduced recombination losses obtained for the proposed device. Accordingly, the quantitative CBO/VBO analysis supports the conclusion that CuGaSe₂ improves the absorber/buffer energetics and contributes to the enhanced *V_{oc}* and reduced recombination of the proposed solar cell.

Under equilibrium conditions, the reference device contains a direct Sb₂Se₃/CdS absorber/buffer interface, whereas the proposed structure introduces CuGaSe₂ between Sb₂Se₃ and CdS. As shown in Fig. 6c,d, this additional absorber layer modifies the local band profile near the front junction region. In the reference structure, the absorber/buffer transition occurs directly at the Sb₂Se₃/CdS interface. In contrast, the proposed structure redistributes this transition across the Sb₂Se₃/CuGaSe₂ and CuGaSe₂/CdS interfaces. This modified band configuration provides a more favorable energetic pathway for electron transport toward the CdS/ZnO front side while maintaining hole selectivity toward the back-contact region. Such an interfacial energy redistribution is consistent with the higher built-in potential extracted from the Mott–Schottky analysis.

Under AM1.5G illumination, the proposed device exhibits a larger separation between the electron and hole quasi-Fermi levels compared with the reference cell, as shown in Fig. 6a,b. This enhanced quasi-Fermi

Interface	χ_A (eV)	χ_B (eV)	$E_{g,A}$ (eV)	$E_{g,B}$ (eV)	$\Delta E_C = E_{C,B} - E_{C,A}$ (eV)	$\Delta E_V = E_{V,B} - E_{V,A}$ (eV)
Sb ₂ Se ₃ /CuGaSe ₂	4.16	4.30	1.10	1.68	−0.14	−0.72
CuGaSe ₂ /CdS	4.30	4.45	1.68	2.42	−0.15	−0.89

Table 7. Calculated conduction-band offset and valence-band offset at the main heterointerfaces of the proposed device.

Interface	N_t (cm ⁻²)	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	η (%)
Sb ₂ Se ₃ /CuGaSe ₂	1×10^{10}	0.775	35.81	70.29	19.51
Sb ₂ Se ₃ /CuGaSe ₂	1×10^{11}	0.775	35.81	70.29	19.51
Sb ₂ Se ₃ /CuGaSe ₂	1×10^{12}	0.775	35.81	70.29	19.51
Sb ₂ Se ₃ /CuGaSe ₂	1×10^{13}	0.774	35.80	70.27	19.46
Sb ₂ Se ₃ /CuGaSe ₂	1×10^{14}	0.763	35.77	70.37	19.20
Sb ₂ Se ₃ /CuGaSe ₂	1×10^{15}	0.728	35.42	69.06	17.82

Table 8. Sensitivity of the proposed Sb₂Se₃/CuGaSe₂ solar cell to the interface defect density (N_t) at the Sb₂Se₃/CuGaSe₂ interface.

Interface	N_t (cm ⁻²)	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	η (%)
CuGaSe ₂ /CdS	1×10^{10}	0.777	35.81	70.80	19.70
CuGaSe ₂ /CdS	1×10^{11}	0.777	35.81	70.75	19.68
CuGaSe ₂ /CdS	1×10^{12}	0.775	35.81	70.29	19.51
CuGaSe ₂ /CdS	1×10^{13}	0.767	35.79	67.53	18.54
CuGaSe ₂ /CdS	1×10^{14}	0.754	35.64	62.56	16.81
CuGaSe ₂ /CdS	1×10^{15}	0.742	35.05	59.64	15.51
CuGaSe ₂ /CdS	1×10^{16}	0.738	34.65	59.23	15.15

Table 9. Sensitivity of the proposed Sb₂Se₃/CuGaSe₂ solar cell to the interface defect density N_t at the CuGaSe₂/CdS interface.

level splitting is directly consistent with the higher open-circuit voltage obtained from the J-V characteristics. Moreover, the modified band bending in the Sb₂Se₃/CuGaSe₂/CdS region supports more efficient carrier separation and reduces the probability of carrier accumulation and recombination near the absorber/buffer interface. Therefore, the band-diagram analysis confirms that CuGaSe₂ does not function only as an additional optical absorber. It also acts as an interfacial energetic modifier that improves band alignment, strengthens carrier selectivity, enhances quasi-Fermi level splitting, and contributes to recombination-loss suppression.

Interface defect density sensitivity analysis

Although the calibrated SCAPS-1D model provides a reliable baseline for evaluating the proposed Sb₂Se₃/CuGaSe₂ dual-absorber architecture, the practical realization of this structure requires careful consideration of non-ideal interfacial defect states. In particular, the insertion of CuGaSe₂ introduces two additional heterointerfaces, namely Sb₂Se₃/CuGaSe₂ and CuGaSe₂/CdS, where defect-assisted recombination may occur. Therefore, to evaluate the robustness of the proposed design, a sensitivity analysis was performed by varying the interface defect density N_t at these two interfaces while keeping all other material and device parameters unchanged. For each N_t value, the J-V characteristics were recalculated and the corresponding V_{oc} , J_{sc} , fill factor, and power conversion efficiency were extracted.

As shown in Table 8, the proposed device exhibits strong tolerance to defect formation at the Sb₂Se₃/CuGaSe₂ interface over a broad range of N_t . When N_t increases from (10^{10}) to (10^{13}) cm⁻², the photovoltaic parameters remain almost unchanged, with the efficiency decreasing only slightly from 19.51 to 19.46%. Even at $N_t = 10^{14}$ cm⁻², the device still maintains an efficiency of 19.20%, indicating that moderate defect densities at the Sb₂Se₃/CuGaSe₂ interface do not severely compromise the performance of the dual-absorber architecture. A more noticeable degradation occurs at $N_t = 10^{15}$ cm⁻², where V_{oc} decreases to 0.728 V and the efficiency decreases to 17.82%. This behavior indicates that excessive interface trap density enhances Shockley-Read-Hall recombination and reduces the quasi-Fermi level splitting, thereby limiting the voltage output and overall efficiency.

Table 9 shows that the CuGaSe₂/CdS interface has a stronger influence on the device performance than the Sb₂Se₃/CuGaSe₂ interface. Up to $N_t = 10^{12}$ cm⁻², the proposed device maintains almost the same performance as the optimized structure, with an efficiency of about 19.51%. However, when N_t increases to 10^{13} cm⁻², the efficiency decreases to 18.54%, mainly due to a reduction in fill factor and V_{oc} . At higher defect densities, the degradation becomes more pronounced. For example, at $N_t = 10^{15}$ cm⁻², V_{oc} , FF, and efficiency decrease to 0.742 V, 59.64%, and 15.51%, respectively. This stronger sensitivity is physically reasonable because the CuGaSe₂/CdS interface is located close to the front junction region, where carrier separation and electron extraction are strongly affected by interfacial recombination.

Overall, the sensitivity analysis confirms that the proposed Sb₂Se₃/CuGaSe₂ architecture is not based solely on an ideal-interface assumption. The device remains highly stable when the defect density at the newly introduced interfaces is kept at or below approximately $10^{12} - 10^{13}$ cm⁻². However, severe degradation occurs at higher

N_t , particularly at the CuGaSe₂/CdS interface. Therefore, future experimental realization of the proposed dual-absorber structure should prioritize passivation and growth control at the CuGaSe₂/CdS front interface, while also maintaining a sufficiently low defect density at the Sb₂Se₃/CuGaSe₂ interface. These results provide realistic interface-quality targets for experimental fabrication and support the physical robustness of the proposed device design.

External quantum efficiency enhancement and comparative absorber response

To clarify the spectral origin of the photocurrent enhancement in the proposed device, the differential external quantum efficiency was calculated as:

$$\Delta EQE(\lambda) = EQE_{\text{Proposed}}(\lambda) - EQE_{\text{Reference}}(\lambda) \quad (19)$$

where EQE_{Proposed} and $EQE_{\text{Reference}}$ denote the wavelength-dependent quantum efficiencies of the Sb₂Se₃/CuGaSe₂ bilayer absorber cell and the reference Sb₂Se₃ cell, respectively. Unlike the absolute EQE spectrum, the differential EQE provides a more direct and quantitative view of the spectral regions in which the proposed architecture contributes to photocurrent enhancement. As shown in Fig. 7a, ΔEQE remains predominantly positive over the investigated wavelength range, confirming that the insertion of the CuGaSe₂ layer does not act as an optical or electrical loss channel. Instead, it improves the photon-to-electron conversion probability over a broad spectral region. The enhancement in EQE can be mathematically expressed by considering the EQE as the product of optical absorption and carrier-collection probability⁴⁶:

$$EQE(\lambda) = A(\lambda)\eta_{\text{col}}(\lambda) \quad (20)$$

where $A(\lambda)$ is the wavelength-dependent absorbance and $\eta_{\text{col}}(\lambda)$ is the carrier-collection efficiency. Therefore, the differential EQE between the proposed and reference cells can be written as:

$$\Delta EQE(\lambda) = A_P(\lambda)\eta_{\text{col,P}}(\lambda) - A_R(\lambda)\eta_{\text{col,R}}(\lambda) \quad (21)$$

or, equivalently,

$$\Delta EQE(\lambda) \approx \eta_{\text{col,R}}(\lambda)\Delta A(\lambda) + A_R(\lambda)\Delta\eta_{\text{col}}(\lambda) + \Delta A(\lambda)\Delta\eta_{\text{col}}(\lambda) \quad (22)$$

where $\Delta A = A_P - A_R$ and $\Delta\eta_{\text{col}} = \eta_{\text{col,P}} - \eta_{\text{col,R}}$. This relation shows that the observed EQE improvement is not necessarily governed by optical absorption alone; it can also originate from improved charge separation, reduced interface recombination, and enhanced carrier collection. This point is particularly important for the present device, because the strongest ΔEQE enhancement occurs in the long-wavelength region, where photons penetrate deeper into the absorber stack and carrier collection becomes more sensitive to the internal electric field, recombination rate, and absorber/junction quality. In the short-wavelength region below approximately 400 nm, the ΔEQE value is relatively small. This behavior is expected because high-energy photons are mostly absorbed close to the front side of the device, where parasitic absorption in the window and buffer layers, as well as surface/interface recombination, can limit the achievable collection gain. However, a clear positive enhancement

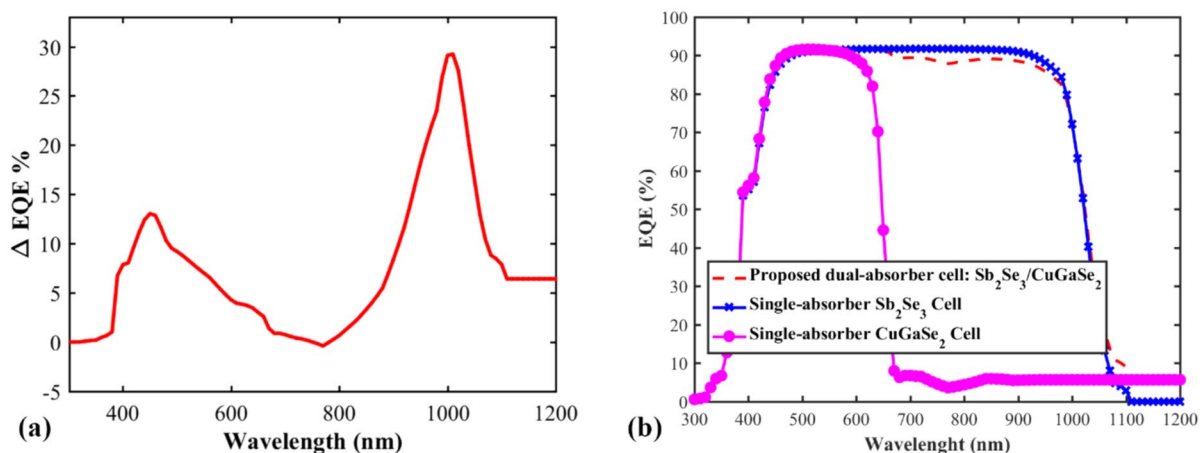


Fig. 7. Spectral response analysis of the proposed Sb₂Se₃/CuGaSe₂ dual-absorber solar cell: **(a)** differential EQE spectrum of the proposed device relative to the reference Sb₂Se₃ cell, defined as $\Delta EQE(\lambda) = EQE_{\text{Proposed}}(\lambda) - EQE_{\text{Reference}}(\lambda)$, and **(b)** comparative EQE spectra of the proposed dual-absorber Sb₂Se₃/CuGaSe₂ cell and the corresponding single-absorber Sb₂Se₃ and CuGaSe₂ cells. The comparative spectra show that CuGaSe₂ mainly contributes to short- and visible-wavelength photon utilization due to its wider bandgap of 1.68 eV, whereas Sb₂Se₃ dominates the long-wavelength and near-infrared response owing to its narrower bandgap of 1.10 eV. Therefore, the proposed device benefits from both modest photocurrent enhancement and, more importantly, improved voltage formation and recombination suppression.

appears around 400–500 nm, reaching approximately 13%. This indicates that the proposed structure improves the utilization of visible photons, most likely through a combination of additional absorption contribution and improved extraction of photogenerated carriers near the front heterointerface.

In the intermediate wavelength region, roughly between 550 and 800 nm, the differential EQE gradually decreases and approaches nearly zero. This suggests that both devices already exhibit comparable carrier-generation and collection capabilities in this spectral range. The absence of a strong negative ΔEQE in this region is important because it confirms that introducing CuGaSe₂ does not significantly compromise the spectral response of the original Sb₂Se₃ absorber. In other words, the CuGaSe₂ interlayer/secondary absorber improves the device response without introducing a severe optical filtering loss in the main visible absorption window.

The most remarkable feature of Fig. 7a, is the pronounced ΔEQE maximum in the near-infrared region, especially around 950–1050 nm, where the enhancement reaches nearly 30%. This long-wavelength improvement is highly significant because photons in this region have lower absorption coefficients and are typically absorbed deeper inside the absorber layer. Therefore, their contribution to EQE is strongly limited by carrier diffusion length, recombination lifetime, depletion width, and the strength of the built-in electric field. The large positive ΔEQE in this region indicates that the proposed Sb₂Se₃/CuGaSe₂ architecture substantially improves the collection of deeply generated carriers. This behavior is consistent with the enhanced V_{oc} , improved fill factor, and higher built-in potential obtained for the proposed device. The contribution of this spectral improvement to the short-circuit current density can be quantified using:

$$\Delta J_{sc} = q \int_{\lambda_1}^{\lambda_2} \Phi_{AM1.5G}(\lambda) \Delta EQE(\lambda) d\lambda \quad (23)$$

where q is the elementary charge and $\Phi_{AM1.5G}(\lambda)$ is the incident photon flux under AM1.5G illumination. Since the experimentally relevant photocurrent is obtained by weighting $\Delta EQE(\lambda)$ with the solar photon flux, the broad positive enhancement between approximately 850 and 1100 nm can make a substantial contribution to the total J_{sc} gain. This explains why the proposed cell exhibits a higher short-circuit current density of 35.80 mA cm⁻² compared with 30.87 mA cm⁻² for the reference cell. Overall, the differential EQE analysis demonstrates that the performance improvement of the proposed device is not a simple consequence of increased absorber thickness. Rather, the spectral redistribution of the quantum-efficiency gain indicates a more effective optoelectronic design, where the CuGaSe₂-assisted architecture enhances carrier collection particularly in the long-wavelength region. This result provides strong evidence that the Sb₂Se₃/CuGaSe₂ bilayer absorber improves both optical utilization and electrical collection, thereby contributing directly to the simultaneous enhancement of J_{sc} , V_{oc} , fill factor, and overall power conversion efficiency.

To further clarify the dual-absorber nature of the proposed Sb₂Se₃/CuGaSe₂ architecture, the EQE response of the proposed bilayer device was also compared with the corresponding single-absorber Sb₂Se₃ and CuGaSe₂ configurations, as shown in Fig. 7b. This comparison provides a clearer distinction between the spectral roles of the two absorber materials and supports the interpretation that the improved response of the proposed device originates from the complementary optical and electronic functions of Sb₂Se₃ and CuGaSe₂.

The single-absorber CuGaSe₂ cell exhibits a strong response mainly in the short- and visible-wavelength region. This behavior is consistent with the wider bandgap of CuGaSe₂, 1.68 eV, which corresponds to an absorption-edge wavelength of approximately 738 nm according to $\lambda_g \approx 1240/E_g$. Therefore, CuGaSe₂ is mainly effective in harvesting higher-energy photons and enhancing carrier generation close to the front junction region. However, its response decreases sharply at longer wavelengths because photons with energies below the CuGaSe₂ bandgap cannot be efficiently absorbed by this layer.

In contrast, the single-absorber Sb₂Se₃ cell shows a broader spectral response extending toward the near-infrared region. This is consistent with the narrower bandgap of Sb₂Se₃, 1.10 eV, corresponding to an absorption edge near 1127 nm. Therefore, Sb₂Se₃ remains the dominant absorber for long-wavelength photon harvesting and near-infrared photocurrent generation. The proposed Sb₂Se₃/CuGaSe₂ dual-absorber cell combines the short-/visible-wavelength contribution associated with CuGaSe₂ and the broad long-wavelength response associated with Sb₂Se₃, resulting in an extended EQE response over a wide spectral range.

It should be emphasized that the improved near-infrared response of the proposed device should not be interpreted as direct near-infrared absorption by CuGaSe₂. Instead, this improvement is mainly attributed to more efficient collection of carriers generated in the Sb₂Se₃ absorber, assisted by the modified absorber/buffer band profile, stronger internal electric field, and reduced recombination losses introduced by the CuGaSe₂ layer. Therefore, Fig. 7b confirms that CuGaSe₂ plays a complementary dual role: it contributes optically to high-energy photon utilization and electronically improves carrier separation and recombination suppression in the Sb₂Se₃-based device.

Although the proposed device exhibits an enhanced short-circuit current density compared with the reference cell, the magnitude of the J_{sc} improvement is more moderate than the increase in V_{oc} . Specifically, J_{sc} increases from 30.87 to 35.80 mA cm⁻², corresponding to an absolute increase of 4.93 mA cm⁻² and a relative enhancement of approximately 16%. In contrast, V_{oc} increases from 0.48 to 0.77 V, corresponding to an absolute enhancement of 0.29 V and a relative increase of about 60%. The fill factor also improves from 67.18 to 70.28%, corresponding to an increase of 3.10 percentage points. As a result, the power conversion efficiency increases from 10.12 to 19.50%, equivalent to an absolute improvement of 9.38 percentage points. These values indicate that the overall efficiency enhancement is primarily governed by the substantial voltage improvement and recombination suppression, while the photocurrent enhancement provides an additional but secondary contribution.

This interpretation is consistent with the comparative EQE spectra shown in Fig. 7b. The single-absorber CuGaSe₂ cell exhibits a strong response mainly in the short- and visible-wavelength region, which agrees with its

wider bandgap of 1.68 eV and corresponding absorption-edge wavelength of approximately 738 nm. Therefore, CuGaSe₂ can directly contribute to high-energy photon absorption and carrier generation near the front-junction region. However, its direct optical contribution at longer wavelengths is limited because photons with energies below the CuGaSe₂ bandgap cannot be efficiently absorbed by this layer.

In contrast, Sb₂Se₃ remains the dominant absorber responsible for long-wavelength and near-infrared photocurrent generation. Its narrower bandgap of 1.10 eV corresponds to an absorption edge near 1127 nm, allowing it to harvest photons over a broader spectral range. Therefore, most of the long-wavelength current in the proposed Sb₂Se₃/CuGaSe₂ device originates from the Sb₂Se₃ absorber rather than from direct CuGaSe₂ absorption.

Accordingly, the role of CuGaSe₂ in the proposed architecture should not be interpreted solely as that of a dominant photocurrent-generating absorber. Instead, CuGaSe₂ provides a combined optical and electronic function. Its direct optical contribution is mainly associated with short- and visible-wavelength photon utilization, while its more significant contribution is electronic: it modifies the absorber/buffer band profile, increases the built-in potential, enhances quasi-Fermi level splitting, and reduces recombination losses. This explains why the improvement in V_{oc} is more pronounced than the improvement in J_{sc} . Therefore, the proposed Sb₂Se₃/CuGaSe₂ device is better described as a dual-absorber and interfacial-energy-engineered architecture, in which Sb₂Se₃ remains the main broadband current-generating absorber and CuGaSe₂ assists both high-energy photon harvesting and recombination suppression.

Generation and recombination profiles

To further clarify the physical origin of the performance enhancement induced by the CuGaSe₂ absorber, the spatial distributions of carrier generation and total recombination were analyzed, as shown in Fig. 8. Figure 8a and b, correspond to the proposed Sb₂Se₃/CuGaSe₂ dual-absorber cell, while Fig. 8c and d, represent the corresponding structure without the CuGaSe₂ layer. The dashed vertical lines indicate the internal interfaces between adjacent layers. Since the photovoltaic output is ultimately governed by the competition between photocarrier generation and recombination loss, this spatial analysis provides deeper insight than the J–V characteristics alone. The local optical generation rate in each absorber can be expressed as⁴⁷:

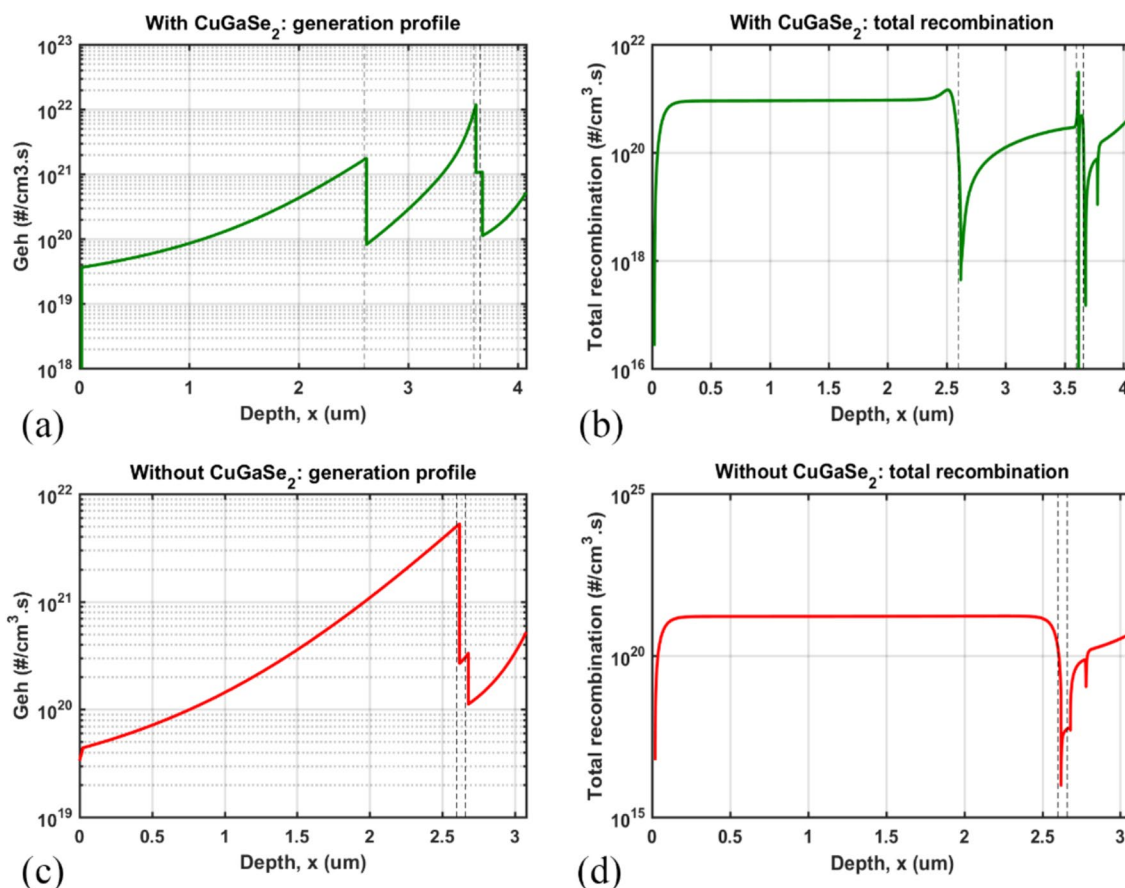


Fig. 8. Spatial distribution of generation and total recombination rates in the devices: (a) generation profile of the proposed Sb₂Se₃/CuGaSe₂ cell, (b) total recombination profile of the proposed cell, (c) generation profile of the reference Sb₂Se₃ cell, and (d) total recombination profile of the reference cell. The insertion of CuGaSe₂ introduces an additional generation-active region and redistributes recombination near the absorber/buffer junction. Dashed vertical lines indicate the material interfaces.

$$G(x) = \int_{\lambda} \alpha(\lambda, x) \Phi(\lambda, x) d\lambda \quad (24)$$

where $\alpha(\lambda, x)$ is the wavelength- and position-dependent absorption coefficient, and $\Phi(\lambda, x)$ is the local photon flux inside the device. In a multilayer absorber, the photon flux reaching a given position is attenuated according to:

$$\Phi(\lambda, x) = \Phi_0(\lambda) \exp \left[- \int_0^x \alpha(\lambda, x') dx' \right] \quad (25)$$

Therefore, the generation profile is strongly affected by both the optical absorption coefficient and the spatial arrangement of the absorber layers. As shown in Fig. 8a, the insertion of CuGaSe₂ introduces an additional generation-active region after the Sb₂Se₃ layer. This additional generation branch is absent in the reference structure without CuGaSe₂, Fig. 8c. The result confirms that CuGaSe₂ does not act as a passive interlayer; rather, it contributes directly to photon harvesting and extends the effective generation volume of the device. A key feature of Fig. 8a, is the step-like redistribution of $G(x)$ at the Sb₂Se₃/CuGaSe₂ interface. This discontinuity is physically expected because the absorption coefficient, bandgap, dielectric response, and optical field distribution change abruptly across the heterointerface. The proposed dual-absorber structure therefore enables photons that are not fully utilized in the Sb₂Se₃ region to be partially absorbed in the CuGaSe₂ layer. In other words, the bilayer absorber increases the probability that transmitted photons are converted into electron–hole pairs before reaching the buffer/window region.

The total recombination rate can be written as the sum of the main recombination channels:

$$R_{\text{tot}}(x) = R_{\text{SRH}}(x) + R_{\text{rad}}(x) + R_{\text{Auger}}(x) \quad (26)$$

where the Shockley–Read–Hall recombination term is given by¹⁴:

$$R_{\text{SRH}} = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \quad (27)$$

The radiative and Auger components are commonly expressed as:

$$R_{\text{rad}} = B(np - n_i^2) \quad (28)$$

$$R_{\text{Auger}} = (C_n n + C_p p)(np - n_i^2) \quad (29)$$

These equations show that recombination is highly sensitive to carrier concentration, defect lifetime, intrinsic carrier density, and interface-induced trap states. Hence, any reduction or spatial redistribution of $R_{\text{tot}}(x)$ can directly improve carrier collection and voltage formation. Figure 8b, shows that, in the proposed Sb₂Se₃/CuGaSe₂ device, recombination is redistributed after the introduction of CuGaSe₂. The recombination rate exhibits strong spatial variation near the internal interfaces, but the important point is that recombination must not be interpreted only from the peak value. For photovoltaic loss analysis, the physically relevant quantity is the spatially integrated recombination:

$$R_{\text{int}} = \int_0^t R_{\text{tot}}(x) dx \quad (30)$$

where t is the total device thickness. A very sharp recombination spike at an interface may appear visually significant on a logarithmic scale, but its contribution to R_{int} can remain limited if it is confined to a narrow spatial region. Therefore, the recombination profile should be assessed through both its magnitude and its spatial width. Compared with the device without CuGaSe₂, Fig. 8d, the proposed structure shows a more controlled recombination distribution around the absorber/buffer region. In the structure without CuGaSe₂, recombination remains strongly concentrated near the absorber junction region, indicating that a considerable fraction of photogenerated carriers is lost before efficient extraction. By contrast, in the dual-absorber configuration, CuGaSe₂ modifies the internal electric-field distribution and provides an additional absorber region that assists carrier separation. This reduces the effective recombination loss associated with the main collection region. This recombination behavior is consistent with the band-diagram analysis in Fig. 6, which shows that the CuGaSe₂ layer modifies the local band bending and interfacial energetics near the absorber/buffer region, thereby supporting reduced carrier loss.

The electrical consequence of this behavior can be understood from the one-dimensional continuity equation:

$$\frac{dJ}{dx} = q [G(x) - R(x)] \quad (31)$$

where J is the carrier current density and q is the elementary charge. After integration over the absorber region, the collected current is governed by the balance between total generation and total recombination:

$$J_{\text{col}} \propto q \int_0^t [G(x) - R(x)] dx \quad (32)$$

This equation clearly demonstrates that an efficient solar cell requires not only high optical generation but also spatial suppression of recombination in regions where photogenerated carriers must be extracted. Therefore, the improvement observed in the proposed device is not simply due to the larger absorber thickness. Instead, it originates from a more favorable balance between generation and recombination.

The advantage of the CuGaSe₂ layer can also be interpreted through a recombination-loss factor:

$$\Gamma_{\text{rec}} = \frac{\int_0^t R_{\text{tot}}(x) dx}{\int_0^t G(x) dx} \quad (33)$$

A lower value of Γ_{rec} indicates that a smaller fraction of the generated carriers is lost through recombination. In the proposed device, the presence of CuGaSe₂ increases the generation-active volume while preventing excessive recombination broadening across the absorber/buffer junction. This improves the net carrier balance and supports the enhancement of J_{sc} , V_{oc} , and fill factor observed in the J–V analysis. Overall, Fig. 8, demonstrates that the CuGaSe₂ layer provides two simultaneous benefits. First, it enhances optical utilization by introducing an additional absorber region capable of generating carriers from photons transmitted through Sb₂Se₃. Second, it modifies the recombination landscape, reducing the effective recombination penalty near the carrier-collection region. This dual optical–electrical role explains why the proposed Sb₂Se₃/CuGaSe₂ architecture outperforms the corresponding structure without CuGaSe₂. The results confirm that CuGaSe₂ is not merely an additional thickness component, but a functional absorber layer that improves photon harvesting, carrier separation, and recombination management.

Thickness-dependent integrated generation and recombination

To quantitatively support the spatial generation–recombination analysis discussed in Fig. 8, 9, summarizes the thickness-integrated and thickness-normalized generation and recombination rates for the devices with and without the CuGaSe₂ absorber layer. This comparison is particularly important because it separates two different physical effects: the contribution of the total absorber volume and the intrinsic recombination tendency per unit thickness. Therefore, Fig. 9, provides a more rigorous basis for evaluating whether the CuGaSe₂ layer merely

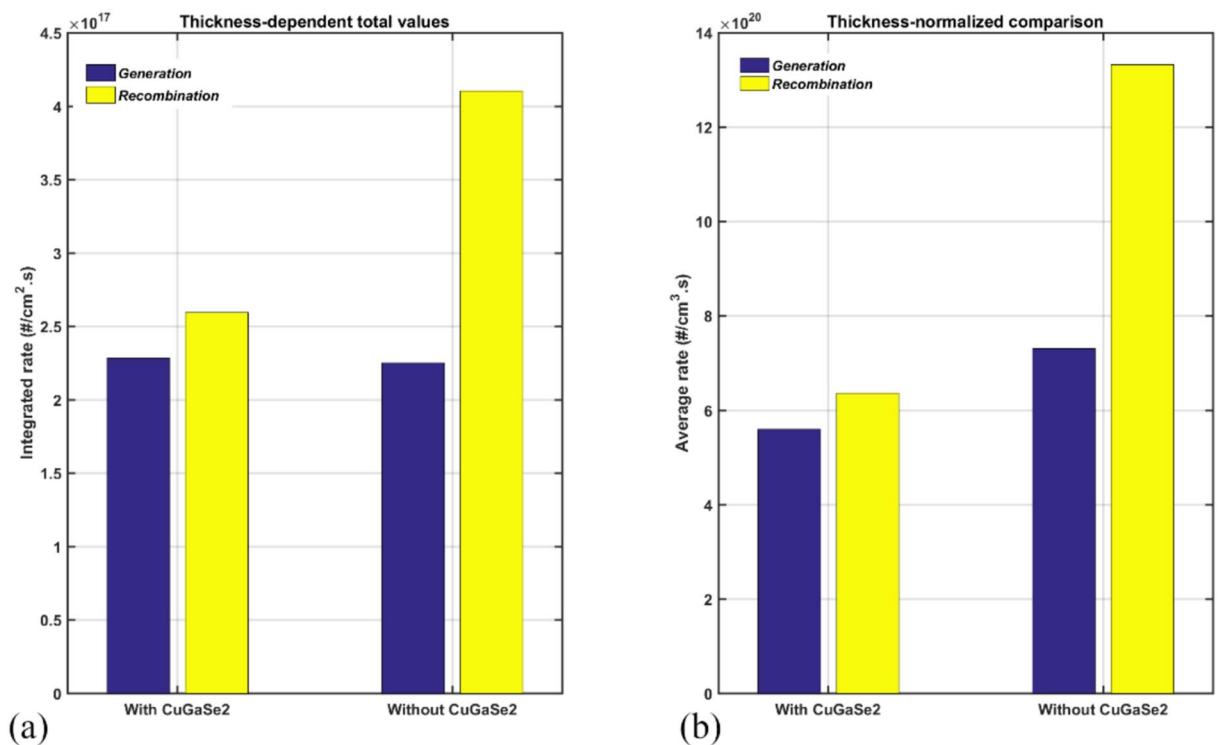


Fig. 9. Comparison of generation and recombination values in the proposed and reference devices: **(a)** thickness-integrated generation and recombination rates and **(b)** thickness-normalized average values. The integrated recombination rate decreases from approximately 4.1×10^{17} to $2.6 \times 10^{17} \text{ cm}^{-2} \text{ s}^{-1}$ after CuGaSe₂ insertion, corresponding to about 36.6% recombination suppression. After thickness normalization, the recombination density decreases from approximately 13.3×10^{20} to $6.4 \times 10^{20} \text{ cm}^{-3} \text{ s}^{-1}$, indicating nearly 52% lower recombination density in the proposed device.

increases the device thickness or truly improves the internal carrier balance. The thickness-integrated generation and recombination rates were calculated as⁴⁵:

$$G_{\text{int}} = \int_0^t G(x) dx \quad (34)$$

$$R_{\text{int}} = \int_0^t R_{\text{tot}}(x) dx \quad (35)$$

where $G(x)$ and $R_{\text{tot}}(x)$ are the local carrier generation and total recombination rates, respectively, and t is the total active device thickness. As shown in Fig. 9a, the integrated generation rate remains almost comparable for the two structures, with only a slight difference between the device with CuGaSe_2 and the device without CuGaSe_2 . This indicates that the improvement in device performance cannot be attributed solely to a trivial increase in the total number of generated carriers. Instead, the dominant difference appears in the recombination channel. The structure without CuGaSe_2 exhibits a much higher integrated recombination rate, approximately $4.1 \times 10^{17} \text{ cm}^{-2} \text{ s}^{-1}$, whereas the proposed dual-absorber structure shows a reduced value of about $2.6 \times 10^{17} \text{ cm}^{-2} \text{ s}^{-1}$. This corresponds to an integrated recombination suppression of approximately:

$$S_R = \left(1 - \frac{R_{\text{int, With CuGaSe}_2}}{R_{\text{int, Without CuGaSe}_2}} \right) \times 100 \quad (36)$$

$$S_R \approx \left(1 - \frac{2.6}{4.1} \right) \times 100 \approx 36.6\% \quad (37)$$

This result is highly significant because it demonstrates that the CuGaSe_2 layer does not introduce an additional recombination burden despite increasing the absorber complexity. On the contrary, it strongly reduces the total recombination loss of the device. Therefore, the performance enhancement of the proposed cell originates not merely from optical absorption extension, but from a more favorable balance between carrier generation and recombination. A more physically meaningful indicator can be obtained by comparing the generation-to-recombination balance:

$$\Psi = \frac{G_{\text{int}}}{R_{\text{int}}} \quad (38)$$

Using the values extracted from Fig. 9a, the proposed device gives approximately:

$$\Psi_{\text{With CuGaSe}_2} \approx \frac{2.3}{2.6} \approx 0.88 \quad (39)$$

whereas the device without CuGaSe_2 gives:

$$\Psi_{\text{Without CuGaSe}_2} \approx \frac{2.25}{4.1} \approx 0.55 \quad (40)$$

Thus, the insertion of the CuGaSe_2 absorber increases the generation-to-recombination balance by nearly:

$$\frac{0.88 - 0.55}{0.55} \times 100 \approx 60\% \quad (41)$$

This improvement is a strong quantitative indication that a larger fraction of the generated carriers can survive recombination and contribute to charge collection in the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ structure. Figure 9b, provides an even stricter comparison by normalizing the generation and recombination rates with respect to the total device thickness⁴⁸:

$$\overline{G} = \frac{1}{t} \int_0^t G(x) dx \quad (42)$$

$$\overline{R} = \frac{1}{t} \int_0^t R_{\text{tot}}(x) dx \quad (43)$$

This normalization removes the direct influence of absorber thickness and allows the intrinsic volumetric behavior of the two devices to be compared more fairly. Interestingly, the thickness-normalized generation rate of the proposed structure is lower than that of the device without CuGaSe_2 . This is expected because the total active region becomes thicker after introducing CuGaSe_2 , causing the generation rate to be distributed over a larger volume. However, the crucial point is that the normalized recombination rate decreases much more strongly than the normalized generation rate. The recombination density decreases from approximately $13.3 \times 10^{20} \text{ cm}^{-3} \text{ s}^{-1}$ in the device without CuGaSe_2 to about $6.4 \times 10^{20} \text{ cm}^{-3} \text{ s}^{-1}$ in the proposed structure, corresponding to a reduction of nearly:

$$\bar{S}_R = \left(1 - \frac{\bar{R}_{\text{With CuGaSe}_2}}{\bar{R}_{\text{Without CuGaSe}_2}}\right) \times 100 \quad (44)$$

$$\bar{S}_R \approx \left(1 - \frac{6.4}{13.3}\right) \times 100 \approx 52\% \quad (45)$$

This result is one of the strongest pieces of evidence supporting the role of CuGaSe₂ as a functional second absorber. Even after removing the thickness effect, the proposed device exhibits nearly half the recombination density of the structure without CuGaSe₂. Therefore, the improvement is not an artefact of using a thicker absorber stack. Rather, it reflects a genuine enhancement in the internal electronic quality of the device. The normalized recombination-to-generation penalty can be expressed as:

$$\rho = \frac{\bar{R}}{\bar{G}} \quad (46)$$

For the proposed cell:

$$\rho_{\text{With CuGaSe}_2} \approx \frac{6.4}{5.6} \approx 1.14 \quad (47)$$

whereas for the structure without CuGaSe₂:

$$\rho_{\text{Without CuGaSe}_2} \approx \frac{13.3}{7.3} \approx 1.82 \quad (48)$$

Thus, the recombination penalty is reduced by approximately:

$$\left(1 - \frac{1.14}{1.82}\right) \times 100 \approx 37\% \quad (49)$$

This reduction directly supports the observed improvement in V_{oc} and fill factor. Since the open-circuit voltage is strongly affected by recombination through the diode saturation current, a lower recombination density reduces non-radiative voltage loss. In simplified form:

$$V_{oc} \approx \frac{kT}{q} \ln \left(\frac{J_{ph}}{J_0} + 1 \right) \quad (50)$$

where J_0 is strongly linked to recombination losses. Therefore, suppressing recombination through CuGaSe₂ insertion lowers the effective recombination current and enables a higher V_{oc} . This explains why the proposed device shows a remarkable voltage improvement compared with the reference configuration. Overall, Fig. 9, provides quantitative evidence that the CuGaSe₂ layer plays a dual role in the Sb₂Se₃-based device. First, it maintains a high integrated generation rate by extending the active photon-harvesting region. Second, and more importantly, it substantially suppresses both integrated and thickness-normalized recombination losses. The reduction of recombination is stronger than any reduction in normalized generation, indicating that the proposed bilayer absorber architecture improves the net carrier balance. Consequently, the enhanced photovoltaic performance of the proposed cell should be attributed not only to additional optical absorption, but also to more efficient recombination management and improved carrier survival within the absorber stack.

Carrier lifetime, diffusion length, and carrier concentration analysis

To further support the interpretation of improved carrier transport and extraction in the proposed device, the effective carrier lifetime, diffusion length, and spatial carrier concentration profiles were analyzed for the reference and Sb₂Se₃/CuGaSe₂ dual-absorber solar cells. Since carrier collection in thin-film heterojunction devices is governed not only by optical generation but also by the ability of photogenerated carriers to survive recombination and reach the selective contacts, these transport-related parameters provide additional insight into the physical origin of the improved photovoltaic performance.

The effective excess-carrier lifetime was estimated from the simulated carrier and recombination profiles according to

$$\tau_{eff} = \frac{\int \delta n_{eff}(x) dx}{\int R_{tot}(x) dx} \quad (51)$$

where $R_{tot}(x)$ is the total recombination rate and $\delta n_{eff}(x)$ represents the effective excess carrier density generated under illumination. The carrier diffusion length was then calculated using

$$L = \sqrt{D\tau_{eff}} \quad (52)$$

where D is the carrier diffusion coefficient. The diffusion coefficient was obtained from the Einstein relation:

Device/region	τ_{eff} (ns)	D_n (cm ² s ⁻¹)	D_p (cm ² s ⁻¹)	L_n (μm)	L_p (μm)
Reference cell/Sb ₂ Se ₃	28	0.388	0.132	1.04	0.61
Proposed cell/Sb ₂ Se ₃ region	46	0.388	0.132	1.34	0.78
Proposed cell/CuGaSe ₂ region	38	2.585	0.646	3.13	1.57

Table 10. Effective carrier lifetime, diffusion coefficient, and diffusion length of the reference and proposed solar cells.

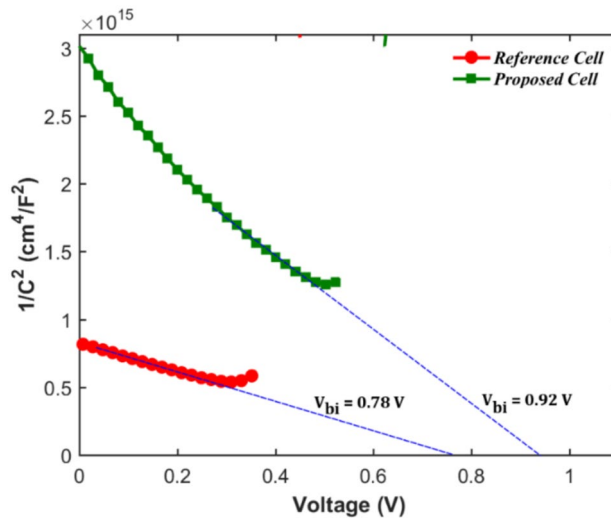


Fig. 10. Mott-Schottky analysis of the reference and proposed solar cells. The built-in potential increases from approximately 0.78 V in the reference Sb₂Se₃ device to about 0.92 V in the proposed Sb₂Se₃/CuGaSe₂ device, corresponding to an enhancement of nearly 18%. The higher built-in potential indicates stronger internal electric-field formation, wider depletion-region behavior, and improved charge-separation capability in the dual-absorber architecture.

$$D = \frac{\mu k_B T}{q} \quad (53)$$

where μ is the carrier mobility, k_B is the Boltzmann constant, T is the temperature, and q is the elementary charge. The extracted effective lifetime and calculated diffusion length values are summarized in Table 10.

As shown in Table 10, the effective carrier lifetime increases from 28 ns in the reference Sb₂Se₃ cell to 46 ns in the Sb₂Se₃ region of the proposed dual-absorber device. This increase indicates that the CuGaSe₂-assisted architecture reduces recombination losses and allows photogenerated carriers to survive for a longer time before recombination. The corresponding electron and hole diffusion lengths in Sb₂Se₃ increase from 1.04 and 0.61 μm to 1.34 and 0.78 μm, respectively. This improvement supports more efficient carrier extraction from the Sb₂Se₃ absorber.

For the CuGaSe₂ region in the proposed device, the effective lifetime is estimated to be 38 ns. Owing to the higher carrier mobilities of CuGaSe₂, the corresponding electron and hole diffusion lengths are 3.13 and 1.57 μm, respectively. These values are larger than the CuGaSe₂ layer thickness of 1.0 μm, indicating that carriers generated within the CuGaSe₂ absorber can be efficiently transported toward the selective contacts before recombination. Therefore, the transport analysis supports the conclusion that CuGaSe₂ contributes not only to short- and visible-wavelength photon absorption, but also to improved carrier separation and extraction.

It should be emphasized that the lifetime and diffusion length values reported here represent effective device-level transport parameters extracted from the calibrated simulation response. They should not be interpreted as intrinsic bulk material constants. Instead, they reflect the combined influence of bulk recombination, interfacial recombination, carrier-selective transport, and electric-field-assisted separation in the complete device.

Built-in potential analysis

To further clarify the electrostatic origin of the performance enhancement, capacitance–voltage analysis was performed using the Mott–Schottky representation, as shown in Fig. 10. The built-in potential was extracted from the linear extrapolation of the $1/C^2$ – V characteristics to the voltage axis. For an abrupt depletion approximation, the Mott–Schottky relation can be expressed as⁴⁹:

$$\frac{1}{C_A^2} = \frac{2}{q\epsilon_s N_{eff}} \left(V_{bi} V \frac{kT}{q} \right), \quad (54)$$

where C_A is the area-normalized capacitance, q is the elementary charge, ϵ_s is the semiconductor permittivity, N_{eff} is the effective ionized defect or doping concentration, V_{bi} is the built-in potential, and V is the applied bias. Therefore, the intercept of the linear region at $1/C^2 = 0$ provides a direct estimate of V_{bi} , while the slope is inversely related to N_{eff} . As observed in Fig. 10, the reference Sb_2Se_3 solar cell exhibits a built-in potential of approximately 0.78 V, whereas the proposed $Sb_2Se_3/CuGaSe_2$ dual-absorber structure shows an increased value of about 0.92 V. This corresponds to an enhancement of nearly 18% in the built-in potential after inserting the $CuGaSe_2$ absorber layer:

$$\frac{0.92 - 0.78}{0.78} \times 100 \approx 17.9\%. \quad (55)$$

This increase is highly significant because V_{bi} governs the strength of the internal electric field across the depletion region. A larger built-in potential promotes more efficient separation of photogenerated electron–hole pairs and reduces the probability of carrier recombination before collection. Therefore, the improvement observed in the J–V characteristics is not only optical in origin but is also strongly supported by enhanced junction electrostatics. The higher $1/C^2$ values of the proposed device also indicate a lower depletion capacitance compared with the reference cell. Since the depletion width is related to capacitance through

$$W = \frac{\epsilon_s}{C_A}, \quad (56)$$

a reduction in capacitance implies a wider space-charge region and a stronger carrier-collection volume. From Fig. 10, the zero-bias $1/C^2$ value of the proposed cell is several times larger than that of the reference device, suggesting a substantially reduced capacitance and a wider depletion region. This wider depletion region is beneficial for absorber-based thin-film solar cells because it allows photogenerated carriers to be separated by the internal field over a longer distance, thereby suppressing bulk recombination and improving charge extraction.

Another important point is the relationship between V_{bi} and the measured open-circuit voltage. The reference device has $V_{bi} \approx 0.78$ V and $V_{oc} \approx 0.48$ V, leaving a voltage deficit of about 0.30 V. In contrast, the proposed cell exhibits $V_{bi} \approx 0.92$ V and $V_{oc} \approx 0.77$ V, reducing this difference to about 0.15 V. This nearly twofold reduction in the electrostatic voltage loss indicates that the proposed $Sb_2Se_3/CuGaSe_2$ architecture converts a larger fraction of the internal built-in potential into usable terminal voltage. This result is consistent with the improved V_{oc} , higher fill factor, and reduced recombination losses discussed in the previous sections. Overall, Fig. 10, provides strong evidence that $CuGaSe_2$ plays a dual role in the proposed device. In addition to extending the optical absorption range, it modifies the internal electric-field distribution and strengthens the junction potential. The higher built-in potential, wider depletion region, and reduced voltage deficit collectively explain the superior charge-separation efficiency and enhanced photovoltaic performance of the proposed dual-absorber solar cell.

Temperature-dependent v_{oc} and activation energy

The temperature dependence of the open-circuit voltage was further analyzed to identify the dominant recombination pathway and to clarify the physical origin of the enhanced photovoltage in the proposed device. Figure 11, presents the variation of V_{oc} with temperature for both the reference and proposed solar cells. For both devices, V_{oc} decreases almost linearly with increasing temperature, which is the expected behavior for recombination-limited thin-film solar cells. However, the proposed $Sb_2Se_3/CuGaSe_2$ dual-absorber device maintains a significantly higher V_{oc} over the entire temperature range, confirming that the $CuGaSe_2$ layer improves not only the optical response but also the internal voltage-building mechanism of the device. The activation energy of recombination was extracted by extrapolating the linear $V_{oc}(T)$ trend to $T = 0$ K. This approach is based on the diode relation under open-circuit conditions,

$$J_{ph} = J_0 \exp \left(\frac{qV_{oc}}{nk_B T} \right), \quad (57)$$

where J_{ph} is the photogenerated current density, J_0 is the reverse saturation current density, n is the ideality factor, k_B is the Boltzmann constant, T is the temperature, and q is the elementary charge. If the saturation current follows an activated behavior,

$$J_0 = J_{00} \exp \left(-\frac{E_a}{k_B T} \right) \quad (58)$$

then the open-circuit voltage can be written as

$$V_{oc}(T) = \frac{E_a}{q} - \frac{nk_B T}{q} \ln \left(\frac{J_{00}}{J_{ph}} \right). \quad (59)$$

Therefore, the intercept of the V_{oc} – T curve at $T = 0$ K gives E_a/q , and the extracted value represents the activation energy associated with the dominant recombination process. As shown in Fig. 11, the reference Sb_2Se_3

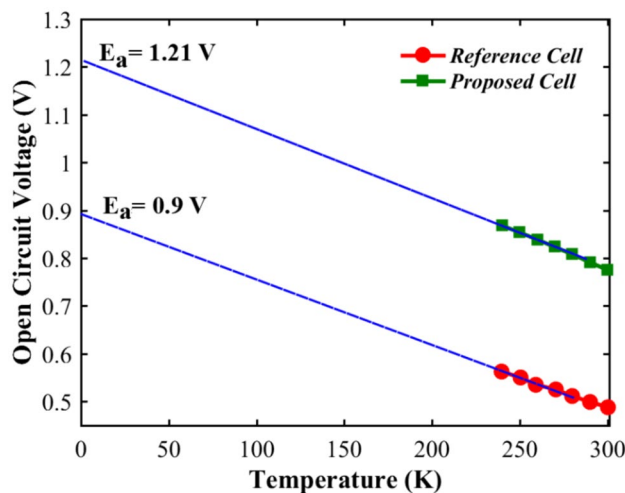


Fig. 11. Temperature-dependent open-circuit voltage of the reference and proposed solar cells and extraction of the recombination activation energy. The activation energy increases from approximately 0.90 eV for the reference Sb_2Se_3 cell to about 1.21 eV for the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ device, corresponding to an enhancement of nearly 34%. The higher activation energy indicates suppression of low-energy defect-assisted recombination pathways and improved absorber/buffer junction quality.

cell exhibits an activation energy of approximately 0.90 eV, whereas the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ device shows a substantially higher value of about 1.21 eV. This corresponds to an activation-energy enhancement of

$$\frac{1.21 - 0.90}{0.90} \times 100 \approx 34.4\%. \quad (60)$$

This increase is highly meaningful because a lower activation energy usually indicates that recombination is dominated by interface-assisted or defect-assisted pathways, where carriers recombine before fully utilizing the absorber bandgap potential. In contrast, the higher activation energy obtained for the proposed device indicates that the dominant recombination channel requires a larger energetic barrier. This suggests that the CuGaSe_2 insertion suppresses low-energy recombination pathways and improves the electronic quality of the absorber/buffer junction. The superiority of the proposed architecture is also evident from the measured operating voltage at room temperature. At around 300 K, the reference cell reaches $V_{oc} \approx 0.49$ V, while the proposed device maintains $V_{oc} \approx 0.78$ V. This represents an increase of nearly 0.29 V, which is consistent with the improved J–V characteristics reported earlier. More importantly, the proposed device converts a larger fraction of its recombination activation energy into usable terminal voltage. The ratio $V_{oc}/(E_a/q)$ increases from approximately

$$\frac{0.49}{0.90} \approx 54.4\% \quad (61)$$

for the reference cell to

$$\frac{0.78}{1.21} \approx 64.5\% \quad (62)$$

for the proposed cell. This improvement indicates that the dual-absorber structure not only raises the energetic ceiling for photovoltage generation but also improves the effectiveness with which the internal potential is converted into external output voltage.

From a device-physics perspective, the higher E_a of the proposed cell confirms that the CuGaSe_2 layer plays a beneficial electronic role beyond simple light absorption. Its insertion modifies the absorber stack, improves carrier separation, and reduces the probability of recombination through energetically shallow defect states. Consequently, the enhanced V_{oc} of the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ solar cell can be attributed to a combination of improved junction energetics, reduced recombination activity, and a higher activation barrier for carrier loss. Therefore, Fig. 11, provides strong evidence that the performance enhancement of the proposed device originates from a genuine improvement in recombination physics rather than from optical current enhancement alone.

Impedance response and charge-transport behavior

A simulated electrochemical impedance spectroscopy was further employed to clarify the charge-transport and recombination behavior of the reference and proposed solar cells. Figure 12, shows the Nyquist plots of both devices, where the real impedance component $\text{Re } Z$ represents the resistive response of the device and the imaginary component $-\text{Im } Z$ reflects the capacitive charge-storage behavior associated with carrier

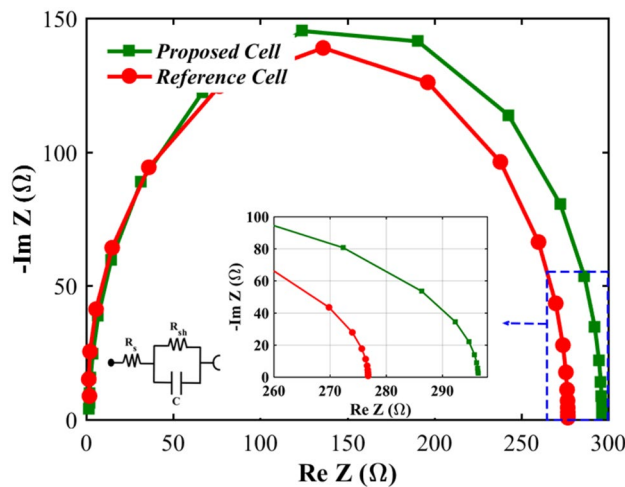


Fig. 12. Nyquist plots and equivalent-circuit analysis of the reference and proposed solar cells. The proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ device exhibits a larger semicircle and a higher low-frequency real-axis intercept, approaching approximately $300\ \Omega$ compared with about $275\text{--}280\ \Omega$ for the reference device. Since the high-frequency intercepts are similar, the enlarged semicircle mainly indicates increased recombination resistance rather than increased series resistance. This confirms reduced recombination loss, improved charge separation, and slower carrier recombination in the proposed dual-absorber device.

accumulation and interfacial polarization. The spectra were interpreted using the equivalent circuit shown in the inset, consisting of a series resistance R_s and a parallel combination of recombination resistance R_{rec} or R_{sh} and capacitance C . In this model, the high-frequency intercept on the real axis corresponds to R_s , whereas the low-frequency intercept is approximately $R_s + R_{\text{rec}}$. Therefore, the diameter of the semicircle directly represents the recombination resistance of the device. For a simplified single-time-constant response, the impedance can be expressed as⁵⁰:

$$Z(\omega) = R_s + \frac{R_{\text{rec}}}{1 + j\omega R_{\text{rec}}C}, \quad (63)$$

where ω is the angular frequency and C is the interfacial or depletion capacitance. Separating the real and imaginary components gives

$$Z' = R_s + \frac{R_{\text{rec}}}{1 + (\omega\tau)^2}, \quad (64)$$

and

$$-Z'' = \frac{\omega\tau R_{\text{rec}}}{1 + (\omega\tau)^2}, \quad (65)$$

where,

$$\tau = R_{\text{rec}}C \quad (66)$$

is the carrier lifetime or relaxation time constant. The maximum of the semicircle occurs when

$$\omega\tau = 1, \quad (67)$$

and at this point,

$$-Z_{\text{max}} = \frac{R_{\text{rec}}}{2}. \quad (68)$$

Thus, a larger semicircle radius and a larger real-axis intercept indicate a higher recombination resistance and a longer carrier lifetime. As observed in Fig. 12, the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ dual-absorber device exhibits a wider Nyquist semicircle than the reference Sb_2Se_3 cell. The low-frequency intercept of the proposed cell shifts toward a higher $\text{Re } Z$ value, approaching approximately $300\ \Omega$, whereas the reference device terminates at a lower value of around $275\text{--}280\ \Omega$. Since the high-frequency intercepts of the two devices are relatively close, the increase in the semicircle diameter cannot be mainly attributed to a higher series resistance. Instead, it reflects an increase in recombination resistance. Using the approximate relation

$$R_{\text{rec}} \approx Z'_{\text{LF}} - Z'_{\text{HF}}, \quad (69)$$

the proposed cell possesses a larger R_{rec} , which confirms that the insertion of CuGaSe₂ suppresses recombination losses rather than introducing an additional resistive transport barrier. This result is highly important because R_{rec} is inversely related to the recombination current. A larger recombination resistance means that photogenerated carriers encounter a weaker recombination pathway before collection. In other words, the CuGaSe₂ layer improves the ability of the device to preserve separated electron–hole pairs. This interpretation is consistent with the higher V_{oc} , improved fill factor, and enhanced activation energy obtained for the proposed cell. Since V_{oc} is strongly governed by recombination according to

$$V_{\text{oc}} \approx \frac{nk_{\text{B}}T}{q} \ln \left(\frac{J_{\text{ph}}}{J_0} + 1 \right), \quad (70)$$

a reduction in the saturation current density J_0 , caused by suppressed recombination, naturally leads to a higher open-circuit voltage. Therefore, the larger semicircle of the proposed device provides direct electrical evidence for the observed voltage enhancement. The inset of Fig. 12, further magnifies the high-resistance region and confirms the same trend. The proposed cell maintains a higher $-\text{Im } Z$ response over a wider $\text{Re } Z$ range, indicating stronger capacitive charge storage and a slower recombination relaxation process. Physically, this means that carriers generated in the Sb₂Se₃/CuGaSe₂ absorber stack remain separated for a longer time before recombination. The improved impedance response can be attributed to the beneficial role of the CuGaSe₂ layer in modifying the absorber/buffer interface, reducing interfacial recombination, and promoting more favorable carrier extraction.

Overall, Fig. 12, provides strong electrical confirmation of the advantage of the dual-absorber architecture. The proposed device does not improve performance only through additional photon absorption; it also improves the internal electronic quality of the solar cell. The increased recombination resistance, enlarged Nyquist semicircle, and enhanced capacitive response demonstrate that the CuGaSe₂ layer effectively suppresses carrier loss pathways and improves charge-collection dynamics. This impedance analysis therefore supports the central conclusion of this work: the Sb₂Se₃/CuGaSe₂ bilayer absorber simultaneously enhances optical generation and reduces recombination losses, leading to the superior photovoltaic performance of the proposed solar cell.

Overall discussion of the performance enhancement mechanism

Based on the combined optical, photovoltaic, capacitance–voltage, temperature-dependent, and impedance analyses, the superior performance of the proposed Sb₂Se₃/CuGaSe₂ solar cell can be attributed to a coupled enhancement mechanism rather than to a single isolated effect. The insertion of the CuGaSe₂ layer fundamentally modifies the absorber architecture by converting the conventional single-absorber Sb₂Se₃ device into a dual-absorber configuration with improved spectral utilization and more favorable internal carrier dynamics. In this structure, CuGaSe₂ serves not merely as an additional light-harvesting layer, but as an active functional component that reshapes the generation–collection balance across the device. From the optical point of view, the CuGaSe₂ layer increases the effective photon-harvesting volume and contributes additional carrier generation in wavelength regions where the reference Sb₂Se₃ device exhibits a comparatively weaker response. This interpretation is supported by the enhanced EQE response and the positive ΔEQE profile, which indicate that the proposed architecture extracts additional photocurrent over a broad spectral range. Importantly, the improvement in J_{sc} is achieved without degrading V_{oc} or FF , confirming that the added absorber does not behave as a parasitic or recombination-dominated layer. Instead, the dual-absorber stack provides a more effective pathway for converting absorbed photons into collected carriers.

The electrical analyses further reveal that the performance gain is strongly associated with improved junction electrostatics and reduced voltage loss. The increase in built-in potential from the reference to the proposed cell indicates stronger internal electric-field formation, which facilitates photogenerated carrier separation and suppresses carrier accumulation near recombination-active regions. This is a critical advantage of the Sb₂Se₃/CuGaSe₂ configuration: the CuGaSe₂ layer improves the device response not only by increasing carrier generation, but also by strengthening the internal driving force required for efficient charge extraction. As a result, the proposed cell maintains a higher current density over a wider voltage range, leading to simultaneous improvements in J_{sc} , V_{oc} , and FF . The proposed mechanism is also supported by the direct band-structure evidence in Fig. 6, where the CuGaSe₂-assisted architecture exhibits improved interfacial energy alignment and larger quasi-Fermi level splitting under illumination.

The recombination-related results provide further evidence for the beneficial role of CuGaSe₂. The generation–recombination analysis shows that the proposed architecture achieves a more favorable balance between carrier generation and recombination, while the thickness-normalized comparison confirms that this improvement is not simply a consequence of absorber-thickness variation. In addition, the higher activation energy extracted from the temperature-dependent V_{oc} analysis suggests that the dominant recombination pathway in the proposed device is less governed by interface-assisted defect recombination. This conclusion is consistent with the impedance analysis, where the larger recombination resistance of the proposed cell indicates slower carrier recombination and improved charge-storage behavior. Therefore, the CuGaSe₂ layer contributes to recombination suppression both through improved energetic alignment and through enhanced carrier-separation dynamics. Overall, the efficiency enhancement from 10.12% in the reference cell to 19.50% in the proposed device results from the synergistic interaction of three key mechanisms: enhanced optical absorption, strengthened internal electric-field-assisted carrier separation, and suppressed recombination losses. The CuGaSe₂ layer therefore acts as a multifunctional absorber modifier rather than a passive secondary absorber. It broadens the photoactive region of the device, improves the internal potential distribution, reduces non-

Research case	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	η (%)	Reference
Simulation	0.77	35.80	70.28	19.50	This work
Experimental	0.48	30.86	67.19	10.12	39
Experimental	0.38	26.24	57.82	5.95	33
Experimental	0.43	25.50	59.33	6.51	51
Experimental	0.32	26.6	43.5	3.92	52
Experimental	0.33	27.69	45.04	4.77	53
Experimental	0.42	29.9	60.4	7.6	54
Experimental	0.40	32.58	70.3	9.2	48
Experimental	0.40	25.14	55.7	5.6	8
Experimental	0.57	10.2	55.3	3.22	26
Experimental	0.39	26.2	57.8	5.93	33
Experimental	0.40	25.69	64.78	6.71	16
Experimental	0.58	33.24	74.63	14.6	55

Table 11. Comparison of V_{oc} , J_{sc} , Fill Factor (FF), and Efficiency (η) values from both experimental and simulation studies.

radiative recombination pathways, and promotes more efficient charge collection. These results demonstrate that $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer absorber engineering is a promising strategy for overcoming the current and voltage limitations of conventional Sb_2Se_3 thin-film solar cells and for advancing their performance toward high-efficiency photovoltaic applications.

Benchmarking with reported Sb_2Se_3 -based solar cells

The photovoltaic performance of the proposed device was further benchmarked against previously reported experimental and simulation-based Sb_2Se_3 solar cells, as summarized in Table 11. This comparison provides a broader context for evaluating the effectiveness of the CuGaSe_2 -assisted bilayer absorber strategy. Since the reported devices were fabricated or simulated under different structural designs, absorber thicknesses, contact configurations, defect densities, and processing conditions, the comparison should not be interpreted as a direct one-to-one assessment. Instead, it serves as a performance benchmark to highlight the potential of the proposed architecture relative to representative Sb_2Se_3 -based solar-cell technologies.

As shown in Table 11, most experimentally reported Sb_2Se_3 solar cells exhibit efficiencies in the range of approximately 3–15%, with performance typically limited by insufficient open-circuit voltage, moderate fill factor, and recombination losses at the absorber/buffer and absorber/back-contact interfaces. In comparison, the proposed device in this work achieves a higher simulated efficiency of 19.5%, accompanied by $V_{oc} = 0.77\text{ V}$, $J_{sc} = 35.80\text{ mA cm}^{-2}$, and $FF = 70.28\%$. The improved J_{sc} indicates that the incorporation of the CuGaSe_2 secondary absorber enhances photon harvesting and carrier generation, while the enhanced V_{oc} suggests reduced voltage loss and more effective suppression of recombination pathways. Moreover, the relatively high fill factor confirms that the additional absorber layer does not introduce a severe transport barrier, but instead contributes to improved charge separation and collection. It is important to emphasize that the performance of the proposed device is obtained from a calibrated SCAPS-1D simulation model, and therefore represents a theoretically achievable performance under the selected material and interface conditions. Nevertheless, the comparison with experimental reports demonstrates that the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer absorber concept can offer a promising route for overcoming the conventional limitations of single-absorber Sb_2Se_3 solar cells. In particular, the simultaneous enhancement of V_{oc} , J_{sc} , and efficiency indicates that CuGaSe_2 acts not only as an additional optical absorption layer, but also as an electrical modifier that improves internal field formation, carrier separation, and recombination resistance. These results suggest that experimental realization of the proposed architecture, together with careful interface engineering and defect control, could provide a viable pathway toward high-efficiency Sb_2Se_3 -based thin-film photovoltaics.

Experimental feasibility and practical fabrication considerations

Although the present study is based on SCAPS-1D simulation, the practical realization of the proposed $\text{Mo}/\text{MoSe}_2/\text{Sb}_2\text{Se}_3/\text{CdS}/\text{ZnO}/\text{Al}/\text{ZnO}$ architecture requires careful consideration of fabrication-related challenges. The simulated efficiency of 19.50% should therefore be interpreted as an achievable device-level target under the selected material, interface, and defect conditions, rather than as an immediately guaranteed experimental value. In particular, the insertion of CuGaSe_2 between Sb_2Se_3 and CdS introduces additional interfaces whose structural and chemical quality will strongly influence the experimentally attainable performance.

A first practical challenge is related to structural mismatch and strain at the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ interface. Sb_2Se_3 is an orthorhombic quasi-one-dimensional chalcogenide absorber, whereas CuGaSe_2 is a tetragonal chalcopyrite semiconductor. Therefore, a fully epitaxial and strain-free interface is not expected in a conventional polycrystalline thin-film stack. Instead, the interface quality will depend on grain orientation, surface roughness, nucleation behavior, and the degree of local structural disorder. Such mismatch can generate interfacial trap states, which may act as Shockley–Read–Hall recombination centers. This issue is directly connected to the interface-defect sensitivity analysis presented in Tables 8 and 9, where the device performance was found to

remain high only when the newly introduced interface defect densities were kept within a moderate range. Therefore, experimental fabrication should prioritize controlled growth of the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ interface and suppression of defect-rich transition regions.

Another important issue is elemental interdiffusion during absorber crystallization and post-deposition annealing. Sb_2Se_3 -based thin-film solar cells often require thermal treatment to improve crystallinity, grain growth, and carrier transport. However, if the CuGaSe_2 and CdS layers are already present during high-temperature processing, interdiffusion may occur at the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ and $\text{CuGaSe}_2/\text{CdS}$ interfaces. Possible Se/S exchange near the $\text{CuGaSe}_2/\text{CdS}$ interface, as well as diffusion of Cu, Ga, Sb, or Cd, could unintentionally modify the absorber composition, local bandgap, doping density, and conduction-band offset. Such changes may disturb the favorable band alignment predicted in the present simulation and increase interfacial recombination. This is particularly important for the $\text{CuGaSe}_2/\text{CdS}$ interface, which was shown to be more sensitive to defect density than the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ interface. Therefore, minimizing interdiffusion and controlling the thermal budget after CuGaSe_2 deposition are essential requirements for experimental realization.

A feasible fabrication route may involve sequential deposition of the multilayer stack under carefully controlled temperature conditions. For example, the Mo back contact can be deposited by sputtering, followed by formation of a thin MoSe_2 interfacial layer through controlled selenization or interfacial reaction. The Sb_2Se_3 absorber may then be deposited using established approaches such as thermal evaporation, vapor transport deposition, close-spaced sublimation, or injection vapor deposition, followed by an optimized crystallization step before the deposition of the CuGaSe_2 layer. CuGaSe_2 can potentially be prepared by sputtering, co-sputtering, thermal evaporation, or selenization-based routes, which are widely used for chalcopyrite-type absorbers. After CuGaSe_2 formation, the subsequent CdS buffer layer should preferably be deposited by a low-temperature chemical bath deposition process to reduce interdiffusion and preserve the intended absorber/buffer band alignment. Finally, ZnO and Al:ZnO layers can be deposited by sputtering as transparent electron-transport and conducting window layers.

Based on the present simulation results, the most critical experimental targets are the control of the $\text{CuGaSe}_2/\text{CdS}$ interface, suppression of interdiffusion during post-deposition processing, and optimization of the CuGaSe_2 thickness and defect density. The interface-defect analysis indicates that maintaining the $\text{CuGaSe}_2/\text{CdS}$ interface defect density at or below approximately 10^{12} – 10^{13} cm^{-2} is important for preserving the predicted performance advantage. Interface passivation, optimized CdS deposition conditions, mild post-deposition annealing, and careful control of the absorber surface before buffer deposition may therefore be necessary. Overall, while the proposed $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ dual-absorber architecture is experimentally challenging, it is physically plausible and provides clear fabrication targets for future experimental validation.

Conclusion

In this work, a CuGaSe_2 -assisted Sb_2Se_3 thin-film solar cell with the configuration $\text{Mo}/\text{MoSe}_2/\text{Sb}_2\text{Se}_3/\text{CdS}/\text{ZnO}/\text{Al:ZnO}$ was proposed and systematically investigated using SCAPS-1D. Prior to evaluating the proposed architecture, the numerical model was calibrated against experimentally reported Sb_2Se_3 solar-cell data. The close agreement between simulation and experiment in terms of J-V behavior, EQE response, integrated photocurrent density, and light-intensity-dependent characteristics confirms the validity of the adopted material parameters and the reliability of the simulation framework.

The introduction of a $1.0 \mu\text{m}$ CuGaSe_2 layer markedly enhanced the photovoltaic performance of the reference Sb_2Se_3 device. The power conversion efficiency increased from 10.12 to 19.50%, while J_{sc} , V_{oc} , and FF improved from 30.87 mA cm^{-2} , 0.48 V, and 67.18% to 35.80 mA cm^{-2} , 0.77 V, and 70.28%, respectively. These improvements demonstrate that the CuGaSe_2 layer functions as an effective secondary absorber, extending the photoactive region, enhancing carrier generation, and improving the generation-collection balance within the device.

Further electrical and recombination analyses revealed that the performance enhancement is not solely optical in origin. The proposed cell exhibited a higher built-in potential, larger activation energy, increased quasi-Fermi level splitting, and higher recombination resistance, indicating stronger internal field formation, reduced voltage losses, and suppressed non-radiative recombination. Overall, the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ bilayer absorber strategy provides a promising route toward high-performance Sb_2Se_3 -based thin-film photovoltaics. Future experimental work should focus on controlled sequential deposition of the $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2/\text{CdS}$ stack, suppression of elemental interdiffusion during thermal processing, passivation of the $\text{CuGaSe}_2/\text{CdS}$ and $\text{Sb}_2\text{Se}_3/\text{CuGaSe}_2$ interfaces, and optimization of the CuGaSe_2 thickness and defect density to validate the predicted device performance and assess the practical applicability of this architecture.

Data availability

All the data, designs, and relevant information associated with this paper are accessible and will be shared upon a reasonable request to the corresponding author.

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Declarations

Competing interests

The authors declare no competing interests.

Ethical approval

The authors confirm that the submitted paper has not been submitted to any other journal and that this version is original and has not been published elsewhere. Additionally, all listed authors affirm the integrity of the study, data, information, and analyses, ensuring that no manipulations have been made. Furthermore, we confirm that no other individuals meet the authorship criteria for this paper beyond those listed as authors.

Additional information

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