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Unfolding the potential of the AgSbSe₂ chalcogenide for advancements in solar cell and photodetector technologies

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The significance of employing a singular, multifunctional material in solar cells and photodetectors has increased due to its substantial impact on device performance. This study presents the design guidelines and an inclusive simulation of high-performance chalcogenide AgSbSe₂-based solar cells and photodetectors using SCAPS-1D for the first time. Through a comprehensive analysis, the potential of multifunctional optoelectronic applications is highlighted by combining an n-CdS window layer with three back surface field (BSF) materials: Al_xGa_{1-x}Sb, FeS₂, and Cu₂SnS₃ (CTS). Among all the examined structures, the n-CdS/p-AgSbSe₂/p⁺-Al_xGa_{1-x}Sb configuration exhibits the highest open circuit voltage (V_{OC}) of 0.85 V and an idealized power conversion efficiency (PCE) of 34.32%, along with a fill factor (FF) of 86.64% and a short circuit current density (J_{SC}) of 46.35 mA cm⁻². Nevertheless, the n-CdS/p-AgSbSe₂/p⁺-FeS₂ and n-CdS/p-AgSbSe₂/p⁺-CTS structures exhibit PCEs of 30.37% and 30.30%, respectively, with the corresponding V_{OC} values of 0.74 V and 0.76 V, underscoring their distinct photovoltaic characteristics. Furthermore, with proper optimization, the AgSbSe₂-based photodetector demonstrates a remarkable responsivity of 0.81 A W⁻¹ and an excellent detectivity of 2.93×10^{15} Jones at a wavelength of 1100 nm. Due to the superior band alignment of n-CdS/p-AgSbSe₂/p⁺-Al_xGa_{1-x}Sb, a higher built-in potential of approximately 2.37 V is achieved by capacitance–voltage (C–V) analysis, which effectively enhances the maximum V_{OC} and overall efficiency of the device.

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1. Introduction

Solar cell technology has emerged as one of the most extensively researched renewable energy sources, attracting significant attention amid the global transition from fossil-based energy systems. To accomplish solar cell objectives, researchers have investigated a variety of solar technologies, such as wafer-based, thin film-based, and organic-based technologies. Solar energy is revolutionized by thin film solar cells because of their incredibly thin, foldable shape and great low-light performance. Although initially limited to laboratory research, crystalline silicon technology has seamlessly transitioned to commercialization and now dominates about 90% of the global solar panel market.¹ In December 2023, LONGI's

heterojunction back contact (HBC) cell achieved an efficiency of 27.09%.² The indirect bandgap of silicon solar cells poses serious constraints since it results in a low absorption coefficient, necessitating the use of thicker wafers for effective light capture. Furthermore, their fabrication is expensive and energy-intensive due to the extraordinarily high temperatures required for their construction, which frequently surpass 1150–2000 °C.³ However, thin film solar cells (TFSCs) have recently attracted substantial research interest because of their cost-effective production, improved structural flexibility, enhanced adaptivity, and perceived high efficiency, which qualify them as an effective substitute for photovoltaic (PV) systems based on silicon.^{4–6} Newly developed thin film photovoltaic materials have shown considerable enhancements in efficiencies. Particularly, CdTe and CIGS solar cells have demonstrated certified PCEs of over 22%.^{7,8} In addition, Sb₂Se₃ and CuInSe₂ solar cells exhibit 10.12% and 15% PCE, respectively.⁹ Despite their optimal efficiency, CdTe and CIGS solar cells are plagued by issues that prevent their large-scale integration. CdTe contains toxic cadmium, posing a threat to the environment, while CIGS relies on rare indium and selenium, driving up production costs. Both of them also degrade more easily than silicon,

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undermining their long-term stability. Therefore, it is important to develop non-toxic chalcogenide and perovskite materials to fabricate solar cells that are both long-lasting and efficient. These materials offer sustainable alternatives to lead-based systems while preserving their advantageous optoelectronic properties, including adjustable bandgaps and high absorption coefficients. Recent studies conducted in 2025 demonstrated that a lead-free CaZrS_3 perovskite can achieve a simulated efficiency exceeding 20%. A separate study on chalcogenide-based materials also showed that $\text{Sb}_2\text{S}_3/\text{SnS}_2$ heterojunctions have perfect band alignment and very little recombination loss, which makes them even more likely to have high theoretical efficiencies.^{10,11} These findings highlight the increased significance of environmentally benign chalcogenides.

In this regard, silver antimony selenide (AgSbSe_2) is an innovative chalcogenide material that demonstrates significant potential and high efficiency. The material exhibits an optimal bandgap and carrier transport characteristics, potentially improving the performance of solar cells. AgSbSe_2 is a p-type semiconductor belonging to the I-V-VI₂ group of chalcogenides.^{12,13} The material has a high absorption coefficient of 10^4 cm^{-1} and a Seebeck coefficient of $320 \mu\text{V K}^{-1}$ at room temperature (300 K).^{13,14} Moreover, recent studies show that the Seebeck coefficient values may be higher than previously thought, reaching about $431\text{--}462 \mu\text{V K}^{-1}$ at higher temperatures.^{15,16} AgSbSe_2 's tunable $\sim 1 \text{ eV}$ bandgap, elevated hole mobility of $1500 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, outstanding electrical mobility, and ultra-low thermal conductivity render it ideally suited for thermoelectric, solar, and optoelectronic applications.^{14,17} Furthermore, silver (Ag) and antimony (Sb) atoms occupy the metal sublattice positions in AgSbSe_2 thin films, which mostly have a cubic crystal structure with the space group $Fm\bar{3}m$. Nevertheless, tetragonal formations have also been observed in this compound.^{13,18} Hence, it is a promising contender for next-generation energy technologies due to its stability, ecological footprint, and compatibility with flexible electronics. Additionally, AgSbSe_2 stands out among chalcogenides due to its unique cubic crystal structure, contrasting sharply with the low-symmetry structures commonly found in many other chalcogenides. Strong structural symmetry yields isotropic electrical and charge-transport characteristics, which are advantageous for uniform carrier collection and permit easier film-orientation criteria in thin-film solar cells. In addition, the symmetric lattice of AgSbSe_2 can accept certain defects, leading to a reduced impact of defect-type variations on its electrical characteristics.^{19,20} Conversely, Sb_2Se_3 possesses a quasi-one-dimensional crystal structure that results in considerable transport anisotropy, rendering the device performance very orientation-dependent.²¹ Besides, Cu_2SnS_3 exhibits significant cation disorder and phase complexity, resulting in major fluctuations in its electrical characteristics and overall performance.²² Meanwhile, AgBiSe_2 comprises bismuth, which raises concerns about its toxicity and phase instability; its electrical characteristics are also markedly sensitive to cation ordering.²³ Although AgSbSe_2 has been extensively studied for

thermoelectric applications, its potential in photovoltaics is mostly unexamined, underscoring the necessity for rigorous exploration in optoelectronic applications.

Furthermore, a few experimental studies have been conducted on AgSbSe_2 PV structures. For example, a fabricated $\text{CdS}/\text{AgSbSe}_2$ device was reported to have a J_{SC} of 0.08 mA cm^{-2} and a V_{OC} of approximately 0.435 V .¹⁴ Additionally, the fabricated $\text{CdS}/\text{Sb}_2\text{S}_3/\text{AgSbSe}_2$ photovoltaic structure exhibited a V_{OC} of 550 mV and a J_{SC} of 2.3 mA cm^{-2} , resulting in a PCE of 0.4% .²⁴ Recently, an AgSbSe_2 -based PV device achieved the best efficiency of 3.51% at low light intensities.²⁵ All the results indicate that the performance levels still fall significantly short of the ideal limit. Consequently, comprehensive investigations must be conducted on AgSbSe_2 to enhance the performance of the AgSbSe_2 -based devices owing to its robust optoelectronic features.

However, a photodetector is an electronic apparatus that facilitates the detection of ultraviolet (UV), infrared (IR), or visible electromagnetic radiation, subsequently converting it into electrical signals.²⁶ Typically operating from visible to near-infrared wavelengths, photodetectors are frequently utilized in optical communication systems, optical interconnections, motion detection, the automobile sector, astronomy and space exploration, and medical imaging.^{27,28} It has been reported that, for visible and near-infrared (NIR) light detection, a bandgap of around 1 eV to 2.5 eV is ideal for photodetection.²⁹ Up to now, most reported photodetectors—such as PbS/TiS_3 , MAPbI_3 , CsPbI_3 , and MoS_2/Si —have exhibited detectivities in the range of 7.5×10^{10} to 3.9×10^{13} Jones and responsivities between 0.3 and 0.6 A W^{-1} .³⁰ However, the instability of perovskite materials limits their practical use; in this regard, AgSbSe_2 , with its suitable bandgap, high responsivity, and excellent electrical properties, has emerged as a promising alternative for photodetector applications.

Besides, there are various methods for depositing AgSbSe_2 thin films, for instance, heating a $\text{Sb}_2\text{S}_3\text{--Ag}$ stack,¹⁷ colloidal synthesis of monodisperse AgSbSe_2 nanocrystals,³¹ hot-injection synthesis of $\text{Sb}_2\text{Se}_3/\text{AgSbSe}_2$ hybrid nanorods,³² and sequential deposition and annealing of polycrystalline AgSbSe_2 .³³ To the best of our knowledge, few studies have been conducted on AgSbSe_2 despite its great potential in photovoltaics. As a consequence, an extensive simulation of AgSbSe_2 is performed in this study to investigate its enormous potential in optoelectronic devices.

In this research, a double heterostructure solar cell and photodetector are utilized, where AgSbSe_2 is employed as the base layer and CdS serves as the window layer, contributing to enhanced device efficiency. CdS is known as an n-type material, and utilizing it as a window layer in a photovoltaic device exhibits power and favourable semiconductor properties for its wider bandgap of 2.4 eV .³⁴

Furthermore, $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$, FeS_2 , and Cu_2SnS_3 have been systematically investigated to assess their suitability and comparative effectiveness as BSF layers in the AgSbSe_2 -based device structures. The ternary alloy $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ is composed of two binary compounds: AlSb and GaSb . This ternary compound has



attracted a lot of attention recently since it can be utilized in sophisticated near- and medium-infrared optoelectronic devices by engineering the band offset and band gap. To date, $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ thin films have been deposited using methods such as molecular beam epitaxy (MBE), liquid phase epitaxy (LPE), and thermal evaporation.³⁵ This ternary alloy has already been utilized as a BSF layer in wafer-based silicon solar cells, and its excellent carrier collection efficiency helps reduce recombination losses.^{35,36} Additionally, the $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ alloy shows promise as a bottom cell absorber in tandem devices.³⁷ However, it may also serve as a viable option for the BSF layer alongside AgSbSe_2 due to its superior band alignment.

Besides, FeS_2 and CTS exhibit direct band gaps of 0.95 eV and 1.07 eV, respectively, and both have identical electron affinities of 4.00 eV.^{35,38} These properties enable them to function effectively as a p^+ -type BSF layer in conjunction with AgSbSe_2 , forming an optimal p/p^+ -heterostructure. In general, the electrically conductive properties and inadequate reflectivity of FeS_2 and CTS are lower than those of traditional BSF materials, like silicon nitride (SiN) or aluminum (Al).³⁹ Moreover, the FeS_2 thin film has garnered considerable attention from the scientific community due to its impressive minority carrier diffusion length, which ranges from 100 to 1000 nm. Additionally, its low cost, non-toxicity, and exceptionally high absorption coefficient (10^5 cm^{-1}) contribute to its appeal.³⁵ The material has previously been used as an absorber layer, achieving an experimental efficiency of only about 3% due to its lower V_{OC} .⁴⁰ However, it may also have the potential to function effectively as a BSF layer when combined with AgSbSe_2 . Besides, CTS is identified as a p-type semiconductor with a variable bandgap ranging from 0.92 to 1.77 eV and an optical absorption coefficient exceeding 10^4 cm^{-1} . Due to these optoelectronic properties, it holds significant potential for applications in visible-light-driven photocatalytic and photovoltaic processes.⁴¹ Experimental studies have indicated a conversion efficiency of approximately 1.35% when CTS is used as the light-absorbing layer.⁴² Additionally, its advantageous band structure and carrier characteristics make it suitable for

forming a p/p^+ junction with AgSbSe_2 , allowing it to function effectively as a BSF layer. This configuration enhances charge confinement and reduces recombination at the rear interface. CTS has recently shown its potential as a BSF layer with CuSbSe_2 in a tandem solar device.⁴³

Therefore, in this study, AgSbSe_2 -based photovoltaic and photodetector devices were systematically designed and analysed in detail. The SCAPS-1D simulation results demonstrate their strong potential for high-performance double heterojunction solar cell applications, as well as their capability to optimize the responsivity and detectivity of AgSbSe_2 for efficient photodetection.

2. Device design and computational approach

Fig. 1(a) indicates the diagrammatic architecture, and 1(b) is the energy band structure of the lighted state for the proposed AgSbSe_2 are both depicted in Fig. 1. In this investigation, CdS is used as a window layer, and $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$, FeS_2 , and CTS are utilized as BSF layers. In this scheme, photons penetrate the window layer of CdS before being observed by AgSbSe_2 . The electron affinity (E.A.) and ionization potential (I.P.) of this p-type AgSbSe_2 layer are 4.12 eV and 5.12 eV, respectively. For the window layer, E_{C} is 4.2 eV and E_{V} is 6.6 eV. The bandgap (E_{G}) and E.A. of the $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ alloy are determined by employing a linear interpolation method between the corresponding values of AlSb and GaSb . The equations below illustrate how the composition of the alloy (X) relates to E_{G} and E.A. according to Vegard's law:³⁷

$$E_{\text{G}_{\text{Al}_x\text{Ga}_{1-x}\text{Sb}}} = X E_{\text{G}_{\text{AlSb}}} + (1 - X) E_{\text{G}_{\text{GaSb}}} \quad (1)$$

$$\text{E.A.}_{\text{Al}_x\text{Ga}_{1-x}\text{Sb}} = X \text{E.A.}_{\text{AlSb}} + (1 - X) \text{E.A.}_{\text{GaSb}} \quad (2)$$

The $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ compound is optimized in this study using eqn (1) and (2), and $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ is identified as the most suitable option for use as a BSF layer with AgSbSe_2 . The

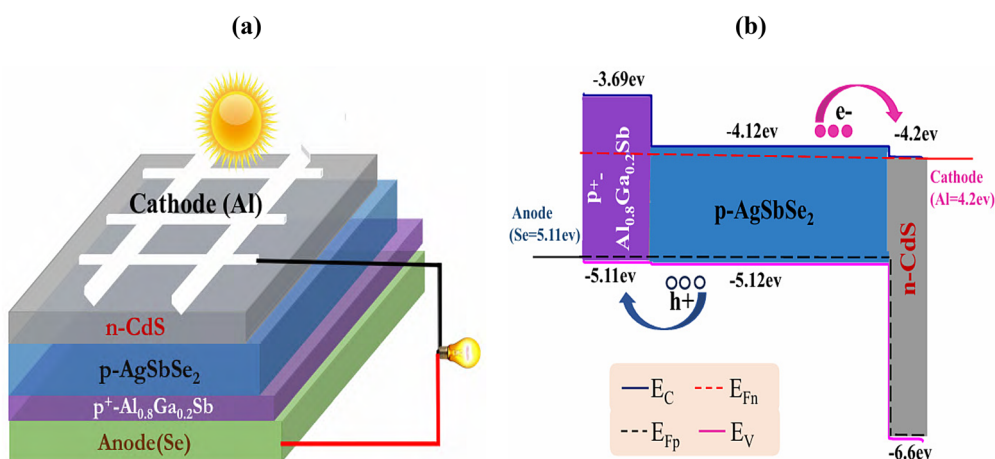


Fig. 1 (a) Methodical design and (b) electronic band layout of the AgSbSe_2 -based device.



bandgap and electron affinity values are considered in this calculation: 0.72 eV and 4.06 eV for GaSb and 1.60 eV and 3.60 eV for AlSb, respectively.³⁷ However, Al_{0.8}Ga_{0.2}Sb alloy shows good band alignment with AgSbSe₂, which makes the junction highly effective.

At the adjacent side, Al_{0.8}Ga_{0.2}Sb, FeS₂, and CTS have E.A. and I.P. of 3.69 eV and 5.11 eV, 4.00 eV and 4.95 eV, and 4.00 eV and 5.07 eV, respectively.^{35,44} These values imply that the heterojunctions formed among the p-type absorber AgSbSe₂, n-type window CdS and p⁺-type BSFs (Al_{0.8}Ga_{0.2}Sb, FeS₂ and CTS) exhibit well-aligned energy bands, promoting efficient charge carrier separation and transport. Moreover, the lattice compatibility analysis indicates that Al_{0.8}Ga_{0.2}Sb (cubic, *a* = 6.13 Å) and FeS₂ (cubic, *a* = 5.4195 Å) have a close lattice match with AgSbSe₂ (cubic, *a* = 5.786 Å), suggesting minimal lattice mismatch and favorable conditions for epitaxial interface formation. In contrast, Cu₂SnS₃ (monoclinic, *a* = 6.653 Å, *b* = 11.537 Å, and *c* = 6.665 Å) displays slightly larger lattice discrepancies; however, its compatible band alignment stability still supports the formation of stable heterojunctions.^{20,36,45,46} In addition to lattice compatibility, these chalcogenides and antimonide compounds exhibit comparable thermal expansion coefficients and demonstrate high phase stability under typical low-temperature processing conditions (less than 350 °C). This reduces the risk of interdiffusion or degradation at the interfaces.⁴⁷ Such favourable structural and thermal compatibility enhances the practical feasibility of integrating AgSbSe₂ with Al_{0.8}Ga_{0.2}Sb, FeS₂, and Cu₂SnS₃ in upcoming experimental implementations.

The illuminated electronic band diagram shown in Fig. 1(b) is drawn considering Al_{0.8}Ga_{0.2}Sb as the BSF layer. Moreover, in Fig. 1(b), the dashed lines labelled as *E_{Fn}* and *E_{Fp}* represent the quasi-Fermi levels of electrons and holes, respectively. The present diagram clearly illustrates that in the window, the *E_{Fp}* is located below the edge of the conduction band (CB), while in the BSF, the *E_{Fn}* is situated above the edge of the valence band (VB). Due to this effect, the electrons generated by light absorption in the absorber layer AgSbSe₂ naturally move toward the window layer CdS, and holes drift to the BSF, facilitating effective carrier transport within the device. Table 1 presents the band offset values for each studied structure. The evaluated conduction band offset (ΔE_C) and valence band offset (ΔE_V) values offer helpful details about interfacial carrier dynamics within the studied heterojunctions. For the CdS/AgSbSe₂ interface, a small ΔE_C (0.08 eV) facilitates smooth electron transport, while a large ΔE_V (1.48 eV) effectively blocks holes, thereby minimizing recombination at the n-type window interface. The AgSbSe₂/FeS₂ (ΔE_C = 0.10 eV, ΔE_V = 0.13 eV) and AgSbSe₂/CTS

(ΔE_C = 0.11 eV, ΔE_V = 0.0488 eV) junctions demonstrate nearly ideal band alignment with minimal energy barriers, which enables balanced carrier transport and efficient current matching between junctions.

Despite a relatively large conduction band offset (ΔE_C = 0.44 eV), the AgSbSe₂/Al_{0.8}Ga_{0.2}Sb interface achieves the highest *V_{OC}* among the structures investigated. This phenomenon can be attributed to the suppression of interfacial recombination due to the higher potential barrier for electron back-transfer, while the minimal ΔE_V (0.02 eV) aids hole transport across the junction. Consequently, the AgSbSe₂/Al_{0.8}Ga_{0.2}Sb heterointerface presents a favourable trade-off between charge selectivity and recombination control, resulting in enhanced *V_{OC}* performance.

The conception of the proposed device in this study is simulated using SCAPS-1D, a one-dimensional solar cell simulation tool often used for analyzing layered semiconductor structures, developed by M. Burgelman and co-workers at the University of Ghent, Belgium.^{48–50} In this model, a bulk defect density of 10¹⁴ cm⁻³ was assigned to the window and BSF layers and 10¹³ cm⁻³ to the absorber layer, which were categorized as either donor or acceptor types based on semiconductor polarity (p-type or n-type) to utilize a Gaussian energy distribution. Moreover, an interface defect density of 10¹⁰ cm⁻² was applied uniformly to each interface of the device due to the lattice mismatch between the different layers. Additionally, the carrier capture cross-sections were established at 10⁻¹⁵ cm² for all layers. As well, 10⁷ cm s⁻¹ was allocated as the thermal velocity for both electrons and holes. To ensure conformity with common real-world photovoltaic performance benchmarks, the simulation was run using conventional test settings, such as an illumination intensity of 1000 W cm⁻² and the AM1.5G sun spectrum. In Table 2, the physical parameters for the window,⁵¹ absorber^{14,17,52,53} and three different BSF layers in detail^{35,44} used in this simulation are shown. Carrier concentrations and overall device behaviour are largely determined by the effective density of states for the valence band *N_V* and the conduction band *N_C*. To ensure precise modelling of the semiconductor properties, these absorber layer parameters were assessed using conventional equations that rely on temperature and the effective masses of electrons and holes.⁴⁴ These values are calculated using the following equations:

$$N_C = 2 \left(\frac{m_c^* K_B T}{2\pi\hbar^2} \right)^{3/2} \quad (3)$$

$$N_V = 2 \left(\frac{m_h^* K_B T}{2\pi\hbar^2} \right)^{3/2} \quad (4)$$

In this work, the effective masses of electrons (*m_c^{*}*) and holes (*m_h^{*}*) in AgSbSe₂ are considered to be 0.26 *m₀* and 1.2 *m₀*, respectively.^{52,54} In addition, *h* is the Planck's constant, *K_B* is the Boltzmann constant, and *T* is the absolute temperature in Kelvin (300 K is used here).

In addition, as the key performance metrics in this investigation, responsivity and detectivity provide a profound

Table 1 Band offset values of all the structures

Junction	ΔE_C	ΔE_V
CdS/AgSbSe ₂	0.08	1.48
AgSbSe ₂ /Al _{0.8} Ga _{0.2} Sb	0.44	0.02
AgSbSe ₂ /FeS ₂	0.1	0.13
AgSbSe ₂ /CTS	0.11	0.0488



Table 2 Material parameters of AgSbSe₂, window and BSF layers incorporated in the simulation

Parameters	n-CdS ⁵¹	p-AgSbSe ₂ ^{14,17,52,53}	p ⁺ -Al _{0.8} Ga _{0.2} Sb ³⁵	p ⁺ -FeS ₂ ³⁵	p ⁺ -CTS ⁴⁴
Bandgap, E_g (eV)	2.40	1.00	1.42	0.95	1.07
Electron affinity, E.A. (χ) (eV)	4.2	4.12	3.69	4.00	4.00
Dielectric permittivity, ϵ (relative)	10.0	7.981	12.04	10.0	10.00
CB effective density of states, N_C (cm ⁻³)	2.2×10^{18}	3.33×10^{18}	7.8×10^{17}	3×10^{18}	2.2×10^{18}
VB effective density of states, N_V (cm ⁻³)	1.8×10^{19}	3.29×10^{19}	1.8×10^{19}	3×10^{19}	1.8×10^{19}
Mobility of electron, μ_e (cm ² V ⁻¹ s ⁻¹)	100	417.4 ⁵²	200	370	100
Hole mobility, μ_h (cm ² V ⁻¹ s ⁻¹)	2500	1500 ¹⁷	420	70	25
Shallow uniform donor density, N_D (1/cm ³)	1×10^{18}	0	0	0	0
Shallow uniform acceptor density, N_A (1/cm ³)	0	1×10^{19} (ref. 53)	1×10^{19}	1×10^{19}	1×10^{19}

understanding of the effectiveness and sensitivity of the developed photonic device. Both are necessary for assessing and maximizing the overall performance of the photodetector device. These can be determined using the following eqn (5) and (6).^{55,56}

$$\text{Detectivity } (D) = \frac{R}{\sqrt{2 \times j_0 \times q}}, \quad (5)$$

$$\text{Responsivity } (R) = \frac{q \times \eta \times \lambda}{h \times c}, \quad (6)$$

where λ denotes the wavelength, η represents the quantum efficiency (QE), h is Planck's constant, j_0 denotes the dark current, q is the charge of an electron and c denotes the speed of light. The calculated dark current was extremely small, about 2.4×10^{-13} mA cm⁻², which is typical for high quality photodetectors and solar cells.

Besides, the J_{SC} , V_{OC} , FF, and PCE values determine the principal electrical photovoltaic characteristics of a solar cell. J_{SC} represents the maximum current output when the terminals of the solar cell are short-circuited, resulting in a voltage of zero. V_{OC} denotes the maximum voltage measurable across a solar cell under open-circuit conditions, where the current equals zero. Additionally, J_{SC} can be defined based on the light absorption and the probability of collecting carriers.⁵⁷

$$J_{SC} = f_c \int_0^{\lambda_m} q \Phi_{AM1.5G}(\lambda) A^1(\lambda) d\lambda, \quad (7)$$

where A^1 represents the one pass absorption, f_c represents the carrier collecting probability, and $\Phi_{AM1.5G}(\lambda)$ represents the incoming light flux. The relationship between J_{SC} and V_{OC} can be expressed as follows:

$$V_{OC} = \frac{KT}{q} \ln \left(\left(\frac{J_{SC}}{J_0} \right) + 1 \right), \quad (8)$$

where K represents the Boltzmann constant, T denotes the absolute temperature, q denotes the elementary charge, and J_0 denotes the saturation current density. FF can be expressed as

$$FF = \frac{P_{max}}{V_{OC} \times J_{SC}}, \quad (9)$$

where $P_{max} = V_m \times I_m$, and at the maximum power point, V_m is the voltage and I_m is the current.

Moreover, efficiency can be defined as follows:

$$PCE = \frac{J_{SC} V_{OC} FF}{P_{in}} \quad (10)$$

where P_{in} = input power.

3. Results and discussion

3.1. Performance of the CdS/AgSbSe₂ solar cell

This analysis explores how structural and material changes within the AgSbSe₂ absorber and CdS window layer, specifically in terms of width, dopant levels, and intrinsic defect states, impact the electrical performance of the proposed n-CdS/p-AgSbSe₂ heterojunction-based solar configuration.

3.1.1. Role of AgSbSe₂ as an absorber layer. Fig. 2 provides a visual representation of how altering the thickness and doping concentration of the absorber influences the photovoltaic response, as presented through contour plots. Fig. 2(a) illustrates that J_{SC} exhibits a notable enhancement, increasing from 33.76 mA cm⁻² to 47.43 mA cm⁻² as the absorber thickness is varied from 0.3 μ m to 1.1 μ m. As thickness increases, more photons are absorbed, resulting in elevated electron-hole pair density and a higher photocurrent, which makes the increase in J_{SC} feasible.⁵⁸ However, doping level variations also significantly affect performance, which moderately decreases the value, indicating that increasing free carrier density enhances free-carrier absorption and non-radiative recombination, which reduces the effective current density in this regime.⁵⁹

The variation in V_{OC} corresponding to the changes in absorber width and carrier density is depicted in Fig. 2(b), which reflects the cell's electrical behaviour. The minimum V_{OC} of 0.62 V is observed at a lower thickness of 0.3 μ m and a concentration of 1×10^{16} cm⁻³ doping levels, indicating that optimal doping levels are critical to maintaining higher voltage outputs. V_{OC} remains nearly constant with increasing thickness at this doping level. In contrast, a noticeable increase in V_{OC} is observed with higher doping concentrations. A peak V_{OC} of 0.67 V is achieved at an absorber thickness of 1.1 μ m combined with a doping concentration of 1×10^{20} cm⁻³. An increase in absorber thickness within the tested range has a negligible effect on V_{OC} , while it increases with higher doping concentration as a result of improved built-in potential and reduced recombination losses.⁶⁰



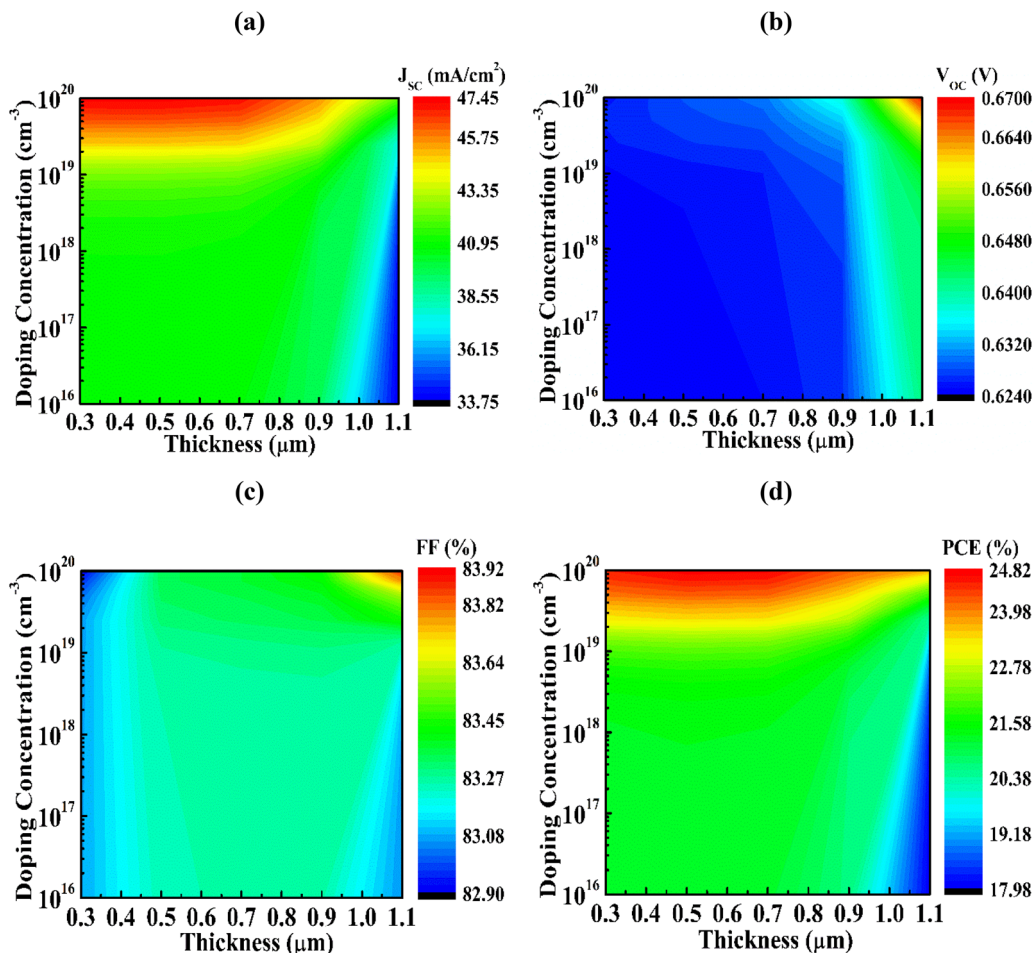


Fig. 2 Analyses of the (a) J_{sc} , (b) V_{oc} , (c) FF, and (d) PCE of the CdS/AgSbSe₂ PV device in accordance with the thickness and doping of AgSbSe₂.

As shown in Fig. 2(c), both the greater thickness and higher doping concentration of the AgSbSe₂ absorber contribute to maintaining a stable FF. Along the thickness range from 0.3 μm to 1.1 μm , FF shows minimal sensitivity, which is only a small variation from 83.06% to 82.9%. However, it slightly increases to 83.92% at the highest doping level of 10^{20} cm^{-3} due to the drops in the ideality factor.⁶¹ Fig. 2(d) depicts that with a thickness of 0.3 μm , PCE is approximately 21.16%. As the thickness attains 1.1 μm with a doping concentration of 10^{17} cm^{-3} , PCE reaches a maximum value of 24.82%. Meanwhile, a substantial increase in doping density from 10^{16} cm^{-3} to 10^{20} cm^{-3} leads to a reduction in PCE to 23.67% at the same thickness of 1.1 μm .

The contour plots in Fig. 3 systematically illustrate the dependence of key photovoltaic characteristics on variations in both the thickness and intrinsic defect concentration of the absorber, offering insights into their combined influence on device performance. According to Fig. 3(a), J_{sc} remains relatively low at 39.51 mA cm^{-2} for small absorber thicknesses and shows a negligible decrease with variations in bulk defect density. As the thickness increases, J_{sc} begins to rise gradually, reaching a maximum value of 45.50 mA cm^{-2} .

Fig. 3(b) demonstrates a steady increase in V_{oc} with increasing absorber, rising from 0.62 V at 0.3 μm to a peak of 0.63 V at 1.1 μm . However, it remains almost stable with variations in defect density within the range of 10^{11} – 10^{15} cm^{-3} . Despite increasing absorber defect density, V_{oc} remains nearly constant because recombination is dominated by interface or depletion-region effect rather than bulk defects. Since charge generation and collection are unaffected, quasi-Fermi level splitting does not change, resulting in an almost invariant V_{oc} .

In Fig. 3(c), FF remains constant with increasing defect density up to 10^{14} cm^{-3} , attaining its maximum value of 83.43%. After that, FF again starts to fall marginally with bulk defects. However, it exhibits slight growth with the width of the absorber. The variation of FF in accordance with the bulk defects might occur due to the change in the ideality factor.⁶² Fig. 3(d) illustrates that PCE initially increases with absorber thickness, rising from 20.62% at 0.3 μm to a maximum of 24.21% at 1.1 μm ; although at the same thickness, it declines to 24.15% when the defect density increases to 10^{15} cm^{-3} . This demonstrates that while thickness improves performance, high defect density has an adverse effect. The optimized values for the width, carrier level, and defects of AgSbSe₂ are identified as



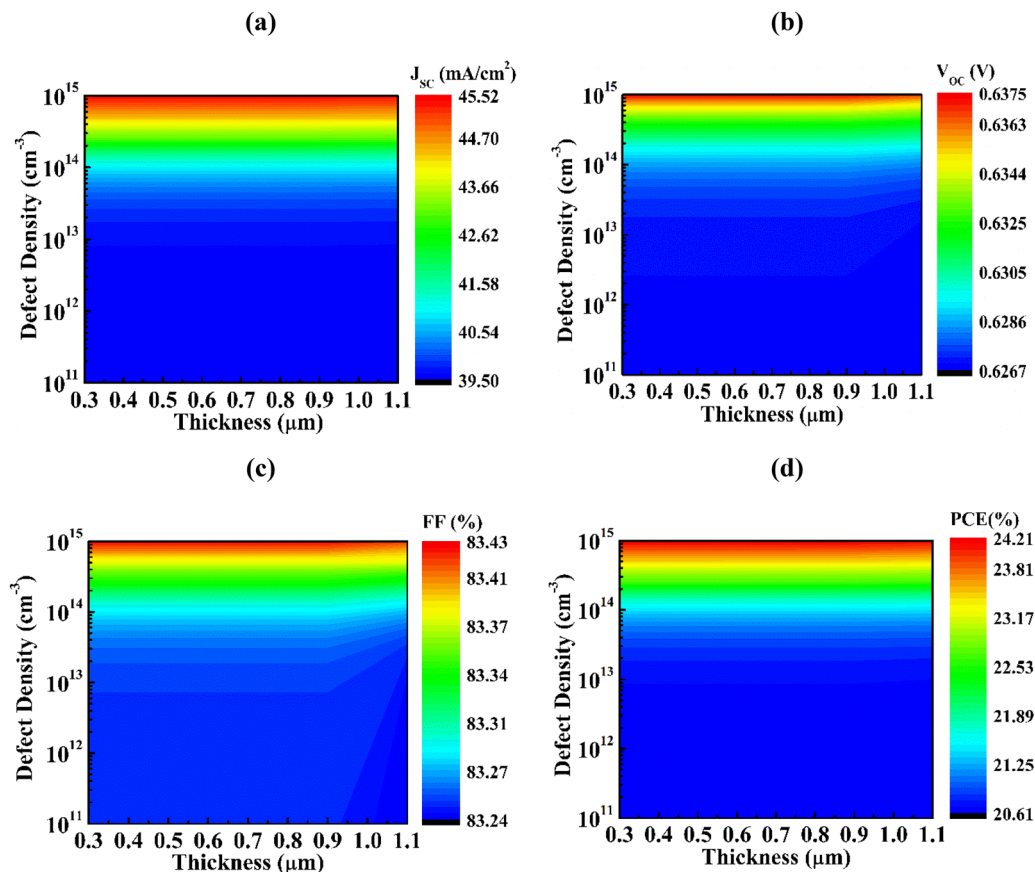


Fig. 3 Analyses of the (a) J_{sc} , (b) V_{oc} , (c) FF, and (d) PCE of the CdS/AgSbSe₂ PV device in accordance with the thickness and defect density of AgSbSe₂.

0.7 μm , 10^{19} cm^{-3} , and 10^{13} cm^{-3} , respectively, for further investigations.

3.1.2. Contribution of CdS as a window layer. From the data depicted in Fig. 4(a), it is clear that adjusting the thickness

within the range of 0.05–0.25 μm of the CdS window layer produces little to no impact on V_{oc} , which remains approximately constant at ~ 0.63 V. This can be explained by the inherent wide bandgap of CdS, which prevents significant

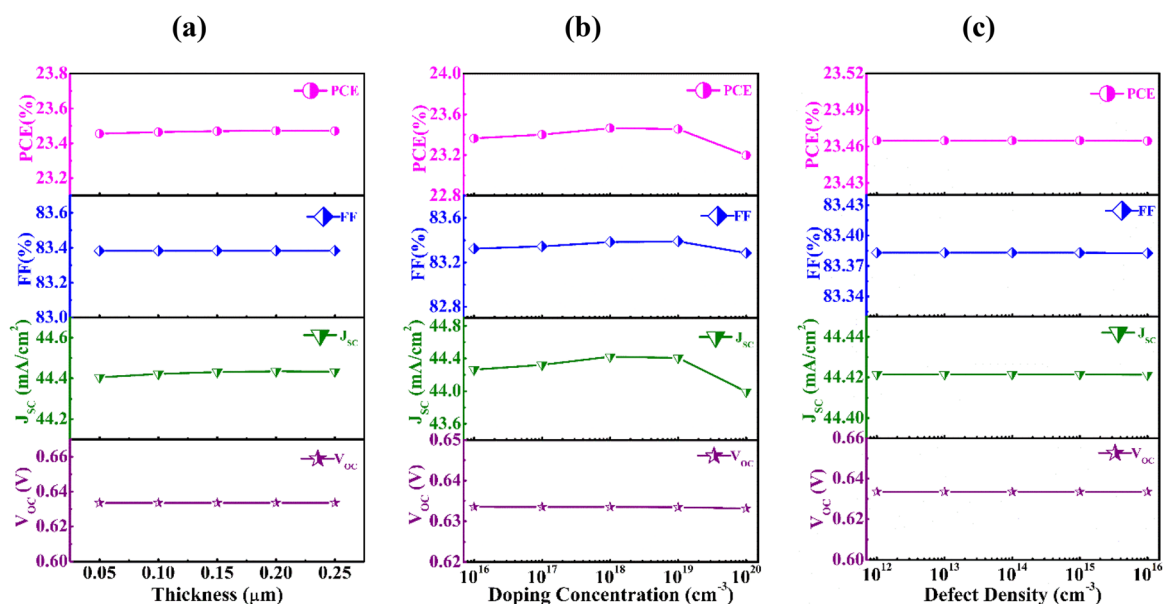


Fig. 4 Photovoltaic performance assessment of the CdS/AgSbSe₂ heterostructure in relation to the (a) width, (b) donor level, and (c) bulk defects of CdS.



absorption losses, thus allowing optimal light penetration to the active region. J_{SC} initially exhibits a value of 44.40 mA cm^{-2} and shows a negligible increase to about 44.43 mA cm^{-2} as the thickness reaches $0.15 \mu\text{m}$. In contrast, PCE and FF remain unaffected by the variation in thickness, maintaining values of approximately 23.4% and 83.38%, respectively. Throughout the investigated thickness range, the CdS window layer exhibits a high carrier lifetime and diffusion length. Because of this trait, electrons can quickly reach the cathode before they recombine, which keeps the device working properly.⁶³

Fig. 4(b) shows the influence of varying CdS doping concentrations from 10^{16} to 10^{20} cm^{-3} on the performance of the n-CdS/p-AgSbSe₂ solar cell. No significant change in V_{OC} is observed here. J_{SC} shows a rising trend as doping concentration increases, up to 10^{19} cm^{-3} due to improved conductivity and enhanced carrier collection. However, at a higher level of 10^{20} cm^{-3} , it drops minimally, which can be attributed to the decreased carrier lifetime. FF exhibits a non-monotonic trend, rising from 83.32% to 83.39% at 10^{19} cm^{-3} , and starts declining from 10^{20} cm^{-3} as a result of enhanced recombination.⁶¹ Here, PCE shows the same behaviour as J_{SC} ; it increases to a level of 10^{19} cm^{-3} , then drops progressively and reaches its lowest point at higher doping levels.

In Fig. 4(c), throughout the CdS layer defect density spanning from 10^{12} to 10^{16} cm^{-3} , the parameters V_{OC} , J_{SC} , FF and PCE maintained stability within the interval values of 0.63 V, 44.42 mA cm^{-2} , 83.38%, and 23.46%, respectively. The CdS window layer's defect density has a limited effect on device performance because of its thin nature and primary role in charge transport rather than carrier generation, resulting in minimal recombination losses despite defect variations. Hence, the most appropriate values for the width, carrier concentration, and defect levels of CdS are determined to be $0.1 \mu\text{m}$, 10^{18} cm^{-3} , and 10^{14} cm^{-3} , respectively, for subsequent studies.

3.2. Performance of the CdS/AgSbSe₂ heterostructures utilizing various BSF layers

In this context, the current–voltage (J – V) characteristic curves of different types of heterostructures with or without a BSF layer are shown in Fig. 5(a), where CdS and AgSbSe₂ are used as window and absorber layers, respectively. Fig. 5(b) illustrates the quantum efficiency (QE) of the same structures, and Fig. 5(c) illustrates the recombination rate. Here, the first figure spells out the values of V_{OC} and J_{SC} measured as 0.6334 V and 44.42 mA cm^{-2} , respectively, without any BSF layer present. After introducing different BSF layers, a noticeable variation in

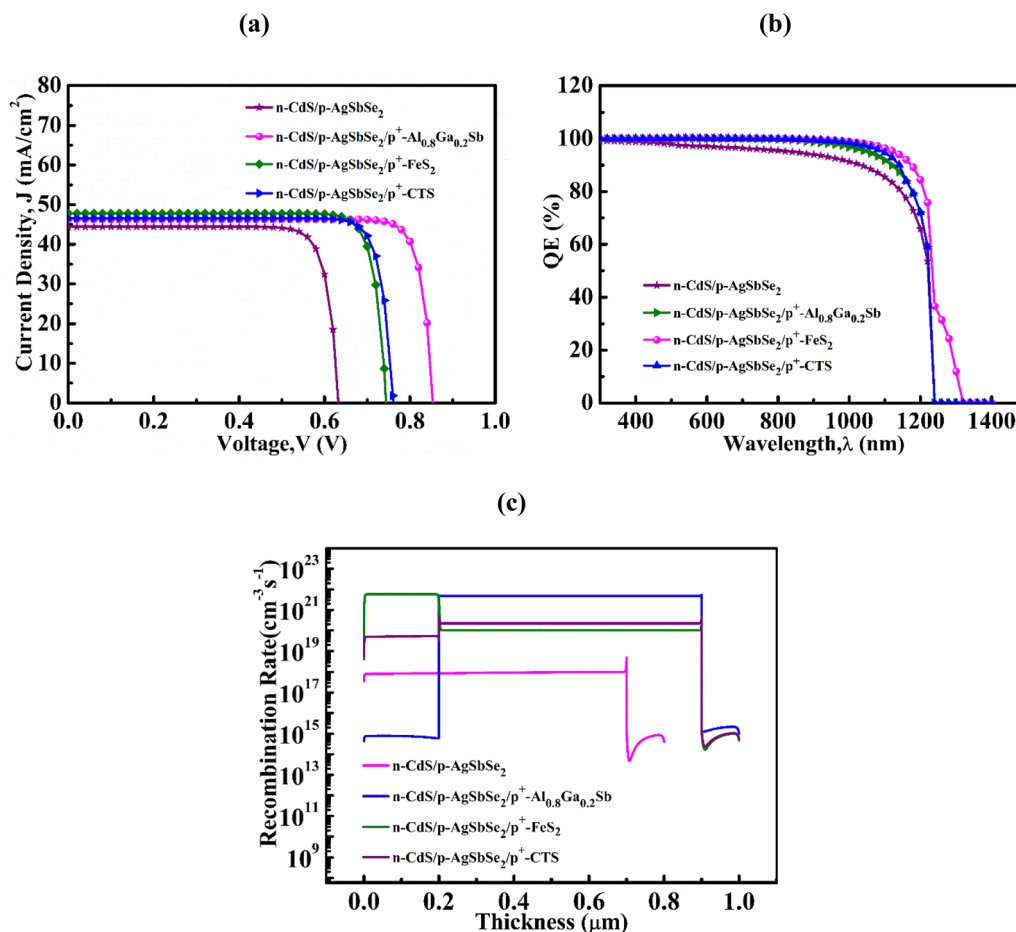


Fig. 5 (a) J – V , (b) QE, and (c) recombination profiles of various AgSbSe₂-based heterostructures.



V_{OC} is observed depending on the band structure of the materials. The simulation parameters for various BSF layers were utilized, as outlined in Table 2. In the dual heterostructure of CdS/AgSbSe₂/FeS₂, there is an appreciable increase in V_{OC} , reaching about 0.74 V, and in CdS/AgSbSe₂/CTS, it becomes 0.76 V. However, the maximum V_{OC} achieved is about 0.85 V at the CdS/AgSbSe₂/Al_{0.8}Ga_{0.2}Sb structure, which can be attributed to the enhanced built-in potential formed at the CdS/AgSbSe₂ and AgSbSe₂/Al_{0.8}Ga_{0.2}Sb heterostructures, highlighting how variations in band alignment across different structures critically influence V_{OC} .⁶⁴ Specifically, the optimal band offset value between AgSbSe₂ and Al_{0.8}Ga_{0.2}Sb increases the built-in potential, contributing to a higher V_{OC} compared to other materials. Besides, the devices with the FeS₂ layer exhibit a considerable improvement in J_{SC} . J_{SC} rises to 46.35 mA cm⁻² at the CdS/AgSbSe₂/Al_{0.8}Ga_{0.2}Sb structure, while the value slightly rises to 46.57 mA cm⁻² in CdS/AgSbSe₂/CTS. The highest J_{SC} of 47.79 mA cm⁻² is shown by FeS₂ compared to the other BSF layers. The constructed current density is elevated by suppressing interface-related carrier recombination, employing the diminution of the surface recombination velocity.⁵⁶

Due to its small bandgap of 0.95 eV, FeS₂ can absorb longer-wavelength photons ranging from 1240 to 1316 nm. This capability contributes to an increase in the current to nearly 1 mA cm⁻² when compared to CTS and Al_{0.8}Ga_{0.2}Sb. The device FF is greatly impacted by the choice of BSF arrangement. The reference n-CdS/p-AgSbSe₂ device shows an FF of 83.38%, while FeS₂ and CTS layers increase FF to 85.30% and 85.49%, respectively, although p⁺ BSFs are preferred for superior performance. The enhanced FF results from increased carrier mobility, longer carrier lifetimes, and decreased recombination, all of which improve carrier collecting efficiency. The slightly higher FF in Al_{0.8}Ga_{0.2}Sb at 86.64% is attributed to ideal band alignment at the absorber and BSF interface, which reduces series resistance and enhances charge transport and diode quality.

In Fig. 5(b), QE is shown with respect to the wavelength. QE measures how effectively a solar cell can transform incoming photons into charge carriers, and its value changes across various wavelengths as a result of the material's absorption properties.⁶⁵ Without the BSF layer, the QE reaches around 99.2% at a wavelength range of 300–360 nm and continuously decreases. Furthermore, at 1240 nm, it becomes zero due to being devoid of photon absorption. When every incoming photon is transformed into electric charges, the maximum photon absorption capability occurs at 100%. After adding the BSF layer, the QE reaches almost 100% in the wavelength range of 300–1000 nm, for all cases. In addition, at 1100 nm, all

of the heterostructures exhibit above 90% QE. However, beyond this point, the QE of the CTS and Al_{0.8}Ga_{0.2}Sb BSF layers drops to zero at 1240 nm, while FeS₂ maintains a non-zero response up to approximately 1316 nm. At a wavelength of 1240 nm, the CdS/AgSbSe₂/FeS₂ device also presents a QE of 35%. This extended absorption range enables FeS₂ to produce an additional photocurrent of around 1 mA compared to the other two BSF-based structures. This suggests that the FeS₂ layer can absorb photons in the 1240–1316 nm range, which contributes to the observed increase of 1 mA in the photocurrent. Hence, it is clear that FeS₂ performs the dual roles of a secondary absorber and a hole transport layer in the AgSbSe₂-based devices.

An inspection of Fig. 5(c) reveals the recombination behaviour of AgSbSe₂ heterostructures incorporating different BSF layers. Recombination is the process by which electrons and holes come together and cancel each other out, which works against the effect of generation. Without a BSF layer, the CdS/AgSbSe₂ setup in the p-region has a very low recombination rate. When a p⁺ layer is added, the recombination rate increases for all structures in the p-region. In addition, FeS₂ exhibits a higher recombination rate within the device compared to CTS and Al_{0.8}Ga_{0.2}Sb in the p⁺-region, resulting in a significantly lower V_{OC} . In contrast, the inclusion of Al_{0.8}Ga_{0.2}Sb as a BSF in the configuration results in the most suppressed recombination rate in the p⁺-region, out of all the examined structures. This reduced recombination facilitates a higher V_{OC} relative to other BSF structures. In AgSbSe₂/Al_{0.8}Ga_{0.2}Sb, the small valence band offset enables efficient hole transport across the junction, while the relatively large conduction band offset serves as an energy barrier that repels electrons from the back contact. This selective carrier confinement significantly reduces interfacial recombination. As a result, the AgSbSe₂/Al_{0.8}Ga_{0.2}Sb configuration promotes better carrier selectivity and enhances V_{OC} by maintaining a high quasi-Fermi level separation near the absorber/BSF interface. As a result, Al_{0.8}Ga_{0.2}Sb is identified as a more favourable BSF material for the AgSbSe₂-based devices. At the same time, CdS serves as an effective window layer for integration with the AgSbSe₂ absorber. However, in the n-region, the recombination rate in FeS₂ devices is notably diminished, and with CTS material designs present, nearly equivalent behaviour is observed due to the small conduction band offset, which facilitates increased electron transport. Conversely, Al_{0.8}Ga_{0.2}Sb shows slightly higher recombination on this side.

The total built-in potential (Ψ_{bi}) of the AgSbSe₂-based double heterostructure PV devices was calculated to assess the internal electric field across the active regions. Table 3 presents the estimated Ψ_{bi} values, derived as the sum of the built-in

Table 3 Variations in the built-in potential of AgSbSe₂ structures with distinct interfaces

Structures		Built-in potential (V)		
n/p	p/p ⁺	n/p	p/p ⁺	Built-in potential (total) (V)
CdS/AgSbSe ₂	AgSbSe ₂ /Al _{0.8} Ga _{0.2} Sb	0.94	1.43	
	AgSbSe ₂ /FeS ₂		0.96	
	AgSbSe ₂ /CTS		1.07	
				2.37
				1.90
				2.01



potentials at the window/absorber (p-n) and absorber/BSF (p-p⁺) junctions:

$$\Psi_{\text{bi}} = \Psi_{(\text{p-n})} + \Psi_{(\text{p-p}^+)} \quad (11)$$

A mathematical expression can be used to determine the built-in voltage in a heterojunction p-n configuration:⁶⁶

$$\psi_{(\text{p-n})} = \frac{\Delta E_{\text{C}} - \Delta E_{\text{V}}}{2q} + \frac{KT}{q} \ln \frac{N_{\text{D}} N_{\text{A}}}{n_{\text{i,n}} n_{\text{i,p}}} + \frac{KT}{2q} \ln \frac{N_{\text{v,n}} N_{\text{c,p}}}{N_{\text{c,n}} N_{\text{v,p}}} \quad (12)$$

where N_{C} and N_{V} denote the density of states of the conduction and valence bands, respectively. E_{C} and E_{V} denote the energy levels at the edges of the conduction and valence bands, respectively. The donor and acceptor doping concentrations are given by N_{D} and N_{A} , respectively. The intrinsic carrier concentrations for the n-type and p-type semiconductors are represented by $n_{\text{i,n}}$ and $n_{\text{i,p}}$. Meanwhile, q denotes the electron charge and KT denotes the thermal energy. The intrinsic carrier concentration (n_{i}) in semiconductors can be calculated from the effective densities of states and the energy gap using a specific exponential formula:⁶⁷

$$n_{\text{i}} = \sqrt{N_{\text{V}} N_{\text{C}}} e^{-\frac{E_{\text{g}}}{2kT}} \quad (13)$$

where E_{g} is the energy bandgap. The provided formula is utilized to determine the potential difference established in $\Psi_{(\text{p-p}^+)}$:⁶⁸

$$\psi_{(\text{p-p}^+)} = \frac{\Delta E_{\text{C}} - \Delta E_{\text{V}}}{2q} + \frac{KT}{q} \ln \frac{N_{\text{A}} N_{\text{A}}}{n_{\text{i,p}} n_{\text{i,p}^+}} + \frac{KT}{2q} \ln \frac{N_{\text{v,p}} N_{\text{c,p}^+}}{N_{\text{c,p}} N_{\text{v,p}^+}} \quad (14)$$

The estimated built-in potential for each interface and total heterostructure is shown in Table 3. The calculated value of Ψ_{bi} for CdS/AgSbSe₂ is 0.94 V. With the incorporation of multiple BSF layers, the voltage increases noticeably, reflecting better charge confinement and improved junction potential. CdS/AgSbSe₂/FeS₂ and CdS/AgSbSe₂/CTS obtain built-in potentials of about 1.90 V and 2.01 V, respectively, which signifies a reduced equilibrium voltage drop across the junction, typically due to a small Fermi level difference between the adjacent layers compared to Al_{0.8}Ga_{0.2}Sb-based BSF. In opposition, CdS/AgSbSe₂/Al_{0.8}Ga_{0.2}Sb provides a maximum built-in potential of about 2.37 V, which leads to attaining the highest V_{OC} . The observed relatively high built-in potential of 2.37 V for this structure is attributed to the significant Fermi level difference between the moderately doped p-type AgSbSe₂ and the highly doped p⁺-type Al_{0.8}Ga_{0.2}Sb. This pronounced doping gradient enhances band bending at the interface, resulting in a stronger internal electric field. Additionally, the small valence band offset facilitates efficient hole transport, while the higher conduction band offset creates a considerable electron barrier that reduces carrier recombination and preserves a strong internal electric field. Collectively, these characteristics contribute to a higher built-in potential compared to other CTS or FeS₂.⁶⁴

3.3. Impact of Al_{0.8}Ga_{0.2}Sb as the BSF layer

The above discussions signify that the Al_{0.8}Ga_{0.2}Sb compounds perform as an optimized BSF layer with AgSbSe₂ absorber layer compared to others. Hence, the subsequent sections discuss the PV results on the AgSbSe₂ solar cells, considering CdS as the window and Al_{0.8}Ga_{0.2}Sb as the BSF layers. Fig. 6 illustrates the

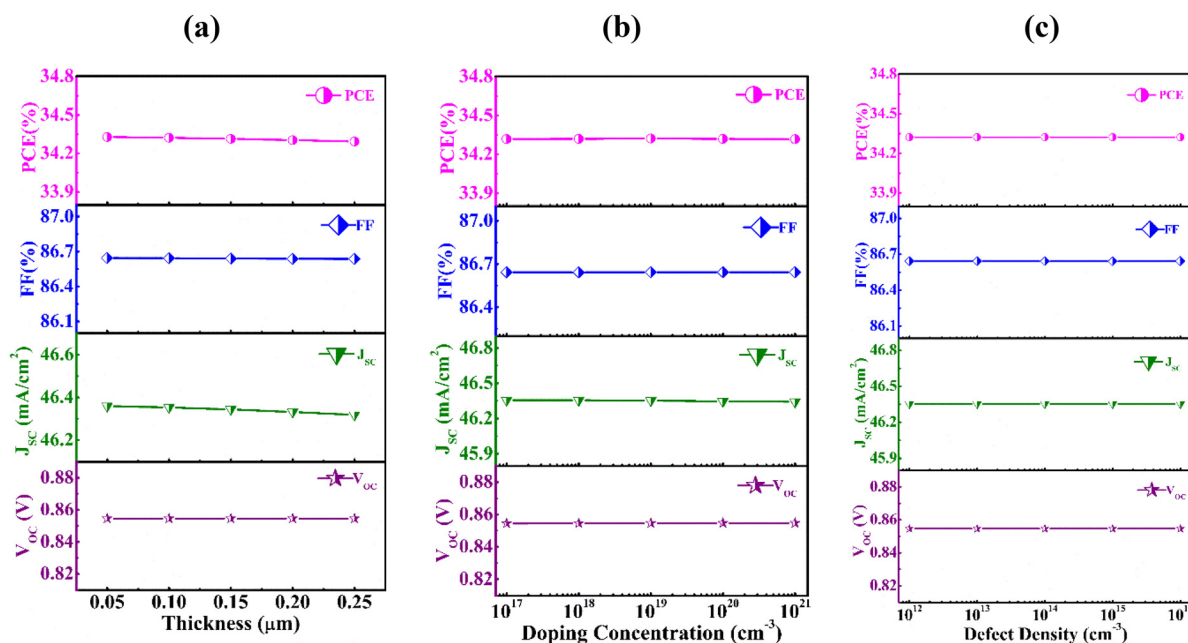


Fig. 6 Photovoltaic performance assessment of the CdS/AgSbSe₂/Al_{0.8}Ga_{0.2}Sb heterostructure in relation to the (a) thickness, (b) acceptor level, and (c) bulk defects of Al_{0.8}Ga_{0.2}Sb.



effect of $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ BSF layer properties, such as thickness, doping level, and defect density, on overall photovoltaic performance. The thickness of the BSF layer is observed in the range of 0.05–0.25 μm , as depicted in Fig. 6(a). In this range, the photovoltaic traits are almost constant: V_{OC} is about 0.86 V, J_{SC} stabilizes at about 46.3 mA cm^{-2} , PCE is around 34.3%, and FF is about 86.6%. This consistency indicates that device performance is not significantly affected by minor variations in BSF thickness, suggesting thickness independence in this interval. Due to the thick electrical confinement and reduced surface recombination, the BSF layer sustains a high carrier lifetime and diffusion length. This allows photogenerated carriers to efficiently reach the hole contact before recombining, thus preserving device performance across the thickness range.

As shown in Fig. 6(b), the PV parameter values here also barely alter when the doping level is changed from 10^{16} to 10^{21} cm^{-3} . J_{SC} and V_{OC} exhibit minimal fluctuations around 46.4 mA cm^{-2} and 0.86 V, respectively, while FF and PCE stay steady near 86.7% and 34.3%. Similarly, under defect density variation, all parameters remain constant and maintain values of V_{OC} around 0.85 V, J_{SC} at 46.35 mA cm^{-2} , FF at 86.6%, and PCE close to 34.3%, as shown in Fig. 6(c).

The stability of observed parameters through all changes in BSF layers demonstrates a regime of material and structural adequacy, where carrier confinement is already optimized, and additional changes become practically ineffective.

3.4. Effect of the absorber's electronic properties on performance

This subsection thoroughly evaluates the effects of defect states, carrier mobility, and band tailing of AgSbSe_2 on n-CdS/p- AgSbSe_2 /p⁺- $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ heterojunction device behaviour.

Fig. 7(a) illustrates how the PV performance of the CdS/ AgSbSe_2 / $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ heterostructure varies in relation to the Urbach energy (U_{E}) states of the AgSbSe_2 absorber layer. The U_{E} indicates the degree of band-tailing and energetic disorder present in the absorber. It primarily influences sub-bandgap absorption and carrier generation. The U_{E} states ranged from 0.02 to 0.1 eV. The figure shows that as the U_{E} of the AgSbSe_2 absorber rises from 0.02 to 0.1 eV, enhanced band-tail absorption allows for better utilization of low-energy photons, leading to an increase in the density of photogenerated carriers. Consequently, J_{SC} has significantly improved. Besides, V_{OC} remains nearly constant because it is governed by quasi-Fermi level splitting, which is primarily influenced by the main recombination pathways. Changes in U_{E} do not significantly affect the primary bulk or interface recombination mechanisms, leading to a saturation current density that remains relatively unchanged. As a result, V_{OC} stays consistent. Additionally, FF is maintained because carrier transport and series resistance do not vary much within the examined range of U_{E} . PCE improves to 36.41% based on the J_{SC} value within the U_{E} range.

Fig. 7(b) examines how all PV responses depend on various defect charge states (neutral, single donor, single acceptor, double donor, double acceptor, amphoteric).

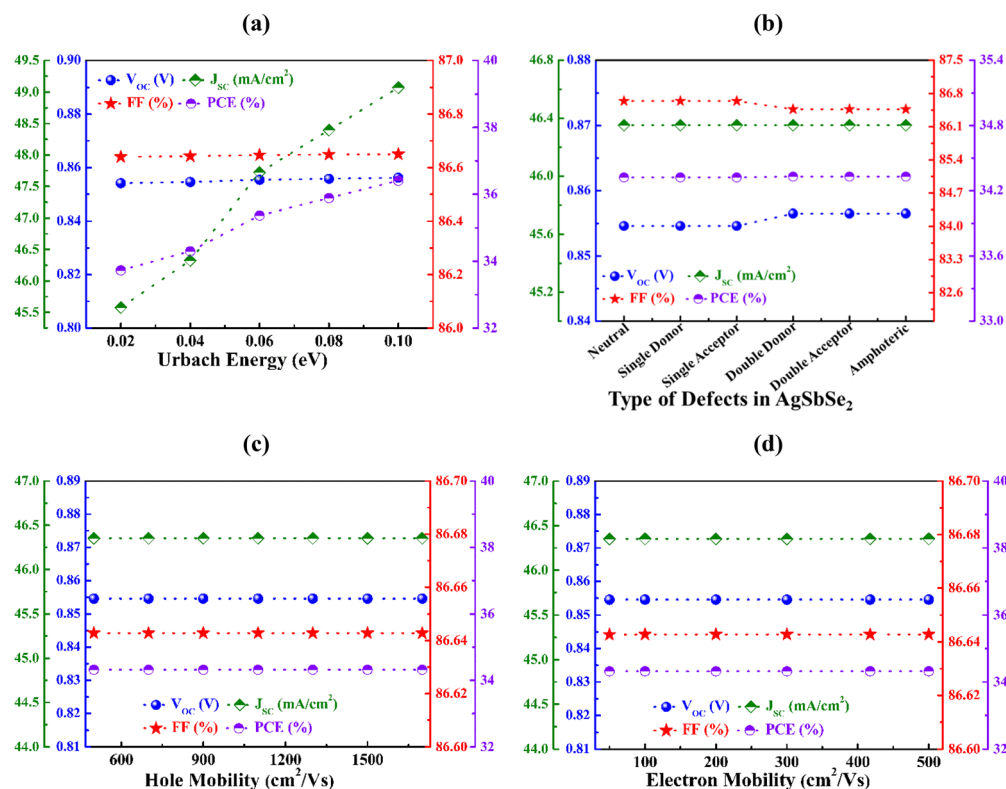


Fig. 7 Photovoltaic performance assessment of the CdS/ AgSbSe_2 / $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ heterostructure in relation to the (a) Urbach energy, (b) defect type, (c) hole mobility, and (d) electron mobility of the AgSbSe_2 absorber.



double donor, double acceptor, and amphoteric) in AgSbSe₂. The figure depicts the almost stable behaviour of all parameters associated with the CdS/AgSbSe₂/Al_{0.8}Ga_{0.2}Sb device. The fact that all PV outputs remain unchanged regardless of the defect charge state (neutral, single donor, single acceptor, double donor, double acceptor, or amphoteric) in the AgSbSe₂ absorber indicates that the electrostatic nature of bulk defects does not constrain the device's performance. Moreover, the various defect states do not significantly alter the carrier lifetime or quasi-Fermi level splitting. This implies that recombination remains governed by processes occurring at the interface or within the depletion region rather than by the charge states of bulk defects.

Fig. 7(c) and (d) illustrate the variation in the photovoltaic (PV) performance of the AgSbSe₂-based device in relation to the hole and electron mobility of the absorber layer, respectively. The hole mobility ranges from 500 to 1700 cm² V⁻¹ s⁻¹, while the electron mobility is adjusted from 50 to 500 cm² V⁻¹ s⁻¹. Both figures demonstrate that the consistency of PV outputs in the proposed heterostructure correlates with the carrier mobility of AgSbSe₂. Changing the mobilities of electrons and holes does not affect the PV parameters, indicating that carrier transport is not the limiting factor in the CdS/AgSbSe₂/Al_{0.8}Ga_{0.2}Sb device. In the range of mobilities examined, the lengths of carrier diffusion exceed the thickness of the absorber. Additionally, the built-in electric field facilitates charge collection and enhances extraction efficiency. Since mobility does not directly influence recombination or quasi-Fermi level splitting, the parameters J_{SC} , V_{OC} , FF, and PCE remain relatively unchanged.

3.5. Effect of device resistances and temperature on device performance

The electrical behaviour of solar cells is greatly influenced by internal series and parallel resistances, which primarily arise due to layer-to-layer contact resistance, electrode interconnections, and structural defects induced during device fabrication.⁶⁹

Performance outcomes in solar cells are strongly influenced by internal resistance elements. The highest PCE is typically attained when the device exhibits minimal series resistance (R_S) and maximized shunt resistance (R_{sh}). This happens because low series resistance reduces power loss in current flow, while high shunt resistance prevents leakage currents, together maximizing the solar cell's output.⁷⁰ Fig. 8 illustrates the variations in R_S , R_{sh} and operating temperature impact the photovoltaic characteristics of the n-CdS/p-AgSbSe₂/p⁺-Al_{0.8}Ga_{0.2}Sb dual-heterojunction solar cell.

Fig. 8(a) illustrates that the FF and PCE of the solar cell decline noticeably as the R_S increases from 0 to 5 Ω cm². In contrast, both V_{OC} and J_{SC} remain largely unaffected by this variation. FF decreases from 86% to 61%. PCE is primarily attributed to the decline in FF; PCE drops from 34.3% to 24.5% as R_S increases within the specified range.

In Fig. 8(b), the solar cell's characteristics shift depending on the applied R_{sh} in the 1–5 kΩ cm² range. Similar to the previous observation for R_S , V_{OC} and J_{SC} remain unaffected by changes in R_{sh} . Both FF and PCE experience a minimal reduction compared to the ideal case when R_{sh} is set to 1 kΩ cm². An increase in R_{sh} leads to higher values of FF and PCE, which reach 86.35% and 34.2%, respectively, at 5 kΩ cm².

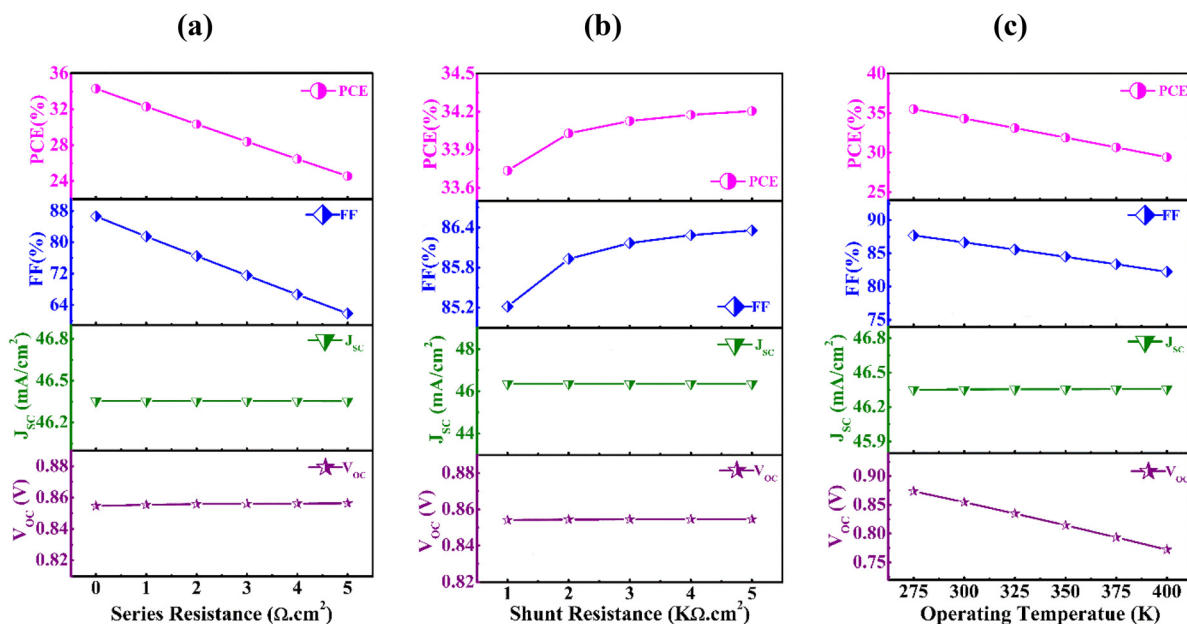


Fig. 8 Photovoltaic performance assessment of the CdS/AgSbSe₂/Al_{0.8}Ga_{0.2}Sb heterostructure in relation to (a) series resistance, (b) shunt resistance, and (c) working temperature.



Fig. 8(c) shows how the solar cell's PV performance changes when the temperature changes between 275 K and 400 K. J_{SC} stays at a fairly steady level in this range of temperature. As the operating temperature rises, V_{OC} drops sharply, from 0.87 V to 0.77 V at 400 K. This decline occurs because the dark current flow increases.²³ The rise in temperature also causes a significant drop in FF, from 87.6% to 82.2%. PCE also undergoes a sharp reduction, dropping to 29.4%, primarily driven by the degradation of V_{OC} and FF across the temperature range. A higher temperature boosts the velocity of charge carriers, which lowers the bond energy and narrows the bandgap of the semiconductor. As a result, the saturation current of the solar cell rises along with the intrinsic carrier concentration.⁷¹

3.6. Efficacy of the AgSbSe₂ absorber in photodetectors

Fig. 9 illustrates how the responsivity and detectivity of the AgSbSe₂ photodetector are influenced by structural changes. This shows that variations in wavelength consistently impact the responsivity and detectivity performance of the device.

As shown in Fig. 9(a), the device without BSF n-CdS/p-AgSbSe₂ exhibits a peak responsivity of 0.76 A W⁻¹ at a wavelength of 1100 nm. In comparison, the inclusion of a BSF layer significantly enhances device performance. Fig. 9(b) to (d) depict the responsivity and detectivity of CdS/AgSbSe₂ devices that incorporate Al_{0.8}Ga_{0.2}Sb, CTS, and FeS₂ BSF layers, respectively. The Al_{0.8}Ga_{0.2}Sb- and CTS-based devices attain peak responsivities of 0.81 A W⁻¹ and 0.84 A W⁻¹, respectively,

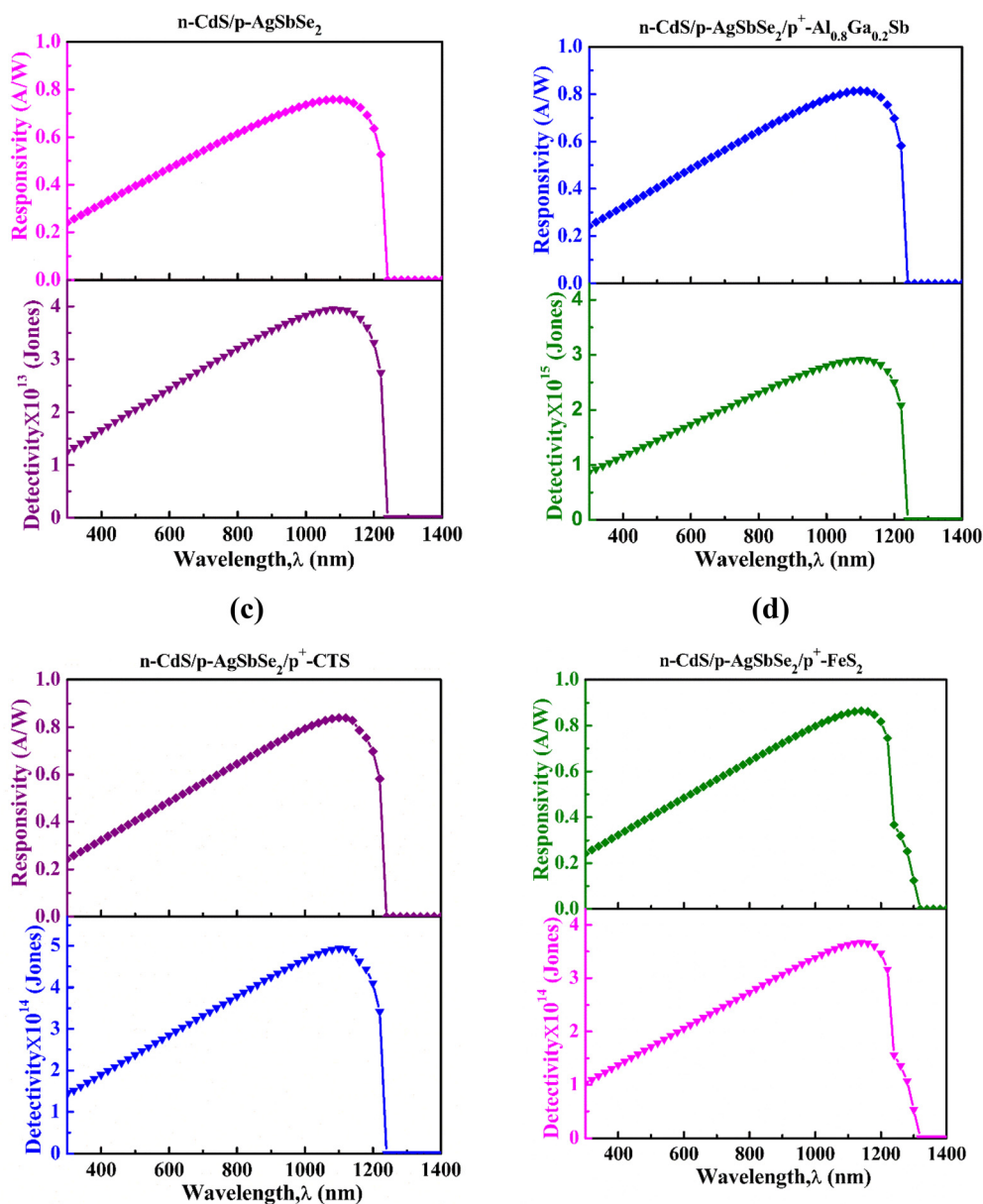


Fig. 9 Detectivity and responsivity performances of the AgSbSe₂-based (a) n-CdS/p-AgSbSe₂, (b) n-CdS/p-AgSbSe₂/p⁺-Al_{0.8}Ga_{0.2}Sb, (c) n-CdS/p-AgSbSe₂/p⁺-CTS, and (d) n-CdS/p-AgSbSe₂/p⁺-FeS₂ photodetectors.



at the same wavelength of 1100 nm, while at the range of 1139 nm, the FeS₂-based structure achieves an improved maximum responsivity of 0.86 A W⁻¹, as displayed in Fig. 9(b)–(d). The incorporation of the BSF layer mitigates recombination, boosts charge carrier concentration and mobility, and enhances carrier collection and current generation, resulting in increased device responsivity.^{30,72} It is also observed that when the wavelength exceeds 1238 nm, the photons no longer carry enough energy to excite electrons, so the photodetector stops responding. However, in this region, FeS₂ generates slightly more current due to its extended absorption range, resulting in relatively higher responsivity up to 1320 nm, beyond which the responsivity drops to zero.

At the same time, the device's detectivity, in the absence of a BSF layer, is 1.24×10^{13} Jones at 300 nm, as shown in Fig. 9(a). It progressively rises to its maximum value of 3.95×10^{13} Jones at 1079 nm. There is a noticeable increase in detectivity after adding a BSF layer. The n-CdS/p-AgSbSe₂/p⁺-Al_{0.8}Ga_{0.2}Sb structure, as presented in Fig. 9(b), exhibits the highest detectivity of any BSF configuration, with a reading of roughly 2.93×10^{15} Jones at 1100 nm and 0.86×10^{15} Jones at 300 nm. This happens because detectivity is inversely dependent on the square root of the dark current; both increasing V_{OC} and lowering the dark current contribute significantly to enhancing the device's detectivity.⁷³ Furthermore, the CTS achieves a detectivity of 4.92×10^{14} Jones at 1100 nm, whereas the FeS₂ layer shows 3.68×10^{14} Jones at 1139 nm, as shown in Fig. 9(c)–(d). These findings demonstrate that improving photodetector performance across many spectral areas requires both absorber thickness and BSF integration. However, detectivity drastically decreases to zero for wavelengths longer than 1236 nm.

3.7. Optimized performances of the AgSbSe₂-based solar cells and photodetectors

An overview of the AgSbSe₂ performance based on both single and double-heterojunction solar cells is illustrated in Table 4. At n-CdS/p-AgSbSe₂ interface, the device exhibits relatively lower performance. With the inclusion of the BSF layer, performance metrics, including V_{OC} , J_{SC} , responsivity, and detectivity, exhibit considerable improvement, thereby validating its role as a key enabling layer for an enhanced optoelectronic response in the device.

It is observed that the highest performance is attained in the dual-heterostructure configuration comprising n-CdS/p-AgSbSe₂/p⁺-Al_{0.8}Ga_{0.2}Sb, as evidenced by a notable PCE of 34.32% and a V_{OC} of 0.85 V. Conversely, the n-CdS/p-AgSbSe₂/p⁺-FeS₂ structure shows a lower PCE of 30.37%, along with a

reduced V_{OC} of 0.74 V. Moreover, the n-CdS/p-AgSbSe₂/p⁺-CTS configuration exhibits a similar PCE of 30.30% and a slightly enhanced V_{OC} of 0.76 V. Although Al_{0.8}Ga_{0.2}Sb provides a better V_{OC} , the FeS₂ BSF shows a higher J_{SC} of 47.79 mA cm⁻². The J_{SC} values for Al_{0.8}Ga_{0.2}Sb and CTS remain closely matched but relatively lower, which are measured at 46.35 and 46.57 mA cm⁻², respectively. FF reaches a maximum value of 86.64% for Al_{0.8}Ga_{0.2}Sb, while FeS₂ and CTS yield slightly lower values of 85.30% and 85.49%, respectively. However, a more recent experimental study reported a PCE of 3.51% for the AgSbSe₂-based devices under low-light conditions.²⁵ In comparison, the simulated double heterostructures presented in this work exhibit superior performance parameters. Since the reported performance of the AgSbSe₂-based optoelectronic devices represents a theoretical and idealized outcome derived from the assumptions inherent in the SCAPS-1D simulation model, the obtained results are likewise idealized. Additionally, in these simulations, optical losses such as reflection at interfaces and parasitic absorption in non-active layers were not explicitly accounted for. Additionally, all layers were assumed to have perfect interfaces and uniform thicknesses. Standard ohmic contacts were established as boundary conditions, and interface defects were included only where explicitly defined, utilizing realistic defect densities from previous studies. Under these idealized conditions, we neglected non-radiative recombination, series and shunt resistances, and other practical device imperfections. Therefore, the reported PCE signifies the upper theoretical limit, providing insights into intrinsic material and layer performance while recognizing that actual devices will encounter further optical and electrical losses.

However, the AgSbSe₂-based photodetector in the absence of any BSF layers leads to a responsivity of 0.76 A W⁻¹. In contrast, this photodetector shows comparable responsivity when integrated with different BSF layers, achieving values of 0.81 and 0.84 A W⁻¹ at 1100 nm for Al_{0.8}Ga_{0.2}Sb and CTS, respectively, with a peak responsivity of 0.86 A W⁻¹ observed for FeS₂ at 1139 nm. Additionally, the reference CdS/AgSbSe₂ device without a BSF layer exhibits a detectivity of approximately 3.95×10^{13} Jones. The detectivities of CdS/AgSbSe₂/CTS and CdS/AgSbSe₂/FeS₂ double heterostructures increase up to the highest 3.68×10^{14} and 4.92×10^{14} Jones, respectively, when CTS or FeS₂ is used as the BSF layer. Notably, the CdS/AgSbSe₂/Al_{0.8}Ga_{0.2}Sb structure achieves the highest detectivity, approaching 2.93×10^{15} Jones. This enhancement can be attributed to the BSF-induced upsurge in the built-in potential, which raises V_{OC} and facilitates efficient carrier separation and collection.

Table 4 Overall cell performances of the AgSbSe₂-based devices

Heterostructures	Solar cell performances				Photodetector performances	
	V_{OC} (V)	J_{SC} (mA cm ⁻²)	FF (%)	PCE (%)	Detectivity (Jones)	Responsivity (A W ⁻¹)
n-CdS/p-AgSbSe ₂	0.63	44.42	83.38	23.46	3.95×10^{13} at $\lambda = 1079$ nm	0.766 at $\lambda = 1100$ nm
n-CdS/p-AgSbSe ₂ /p ⁺ -Al _{0.8} Ga _{0.2} Sb	0.85	46.35	86.64	34.32	2.93×10^{15} at $\lambda = 1100$ nm	0.819 at $\lambda = 1100$ nm
n-CdS/p-AgSbSe ₂ /p ⁺ -FeS ₂	0.74	47.79	85.30	30.37	3.68×10^{14} at $\lambda = 1139$ nm	0.867 at $\lambda = 1139$ nm
n-CdS/p-AgSbSe ₂ /p ⁺ -CTS	0.76	46.57	85.49	30.30	4.92×10^{14} at $\lambda = 1100$ nm	0.842 at $\lambda = 1100$ nm



These findings align well with recently reported dual hetero-junction photodetectors, whose detectivities typically fall in the range of 10^{15} – 10^{18} Jones. For example, $\text{Cu}_2\text{ZnGeSe}_4$ -based devices (I_2 – II – IV – VI_4 family) exhibit a detectivity of 8.28×10^{17} Jones,⁷⁴ ZnGeAs_2 achieves 1.25×10^{17} Jones,⁷⁵ Fe_2GeS_4 reaches 2.74×10^{16} Jones,⁷⁶ and the n-ZnSe/p-CdGeP₂/p⁺-GeS dual heterojunction device attains 3.87×10^{18} Jones.⁷⁷ Moreover, Ag_3AuS_3 - and Ag_3AuSe_2 -based photodetectors have also demonstrated detectivities of the order of 10^{15} Jones.^{73,78} These comparisons confirm that the proposed AgSbSe_2 -based double heterostructures exhibit competitive detectivity performance relative to state-of-the-art chalcogenide and I–III–VI₂ systems.

4. Conclusion

This work successfully reveals the potential of novel AgSbSe_2 -based solar cells and photodetectors through theoretical investigation. This design manifests CdS as a window and $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$, FeS_2 and CTS as BSF layers. The impact of crucial factors such as layer thickness, carrier concentration, and defect density is systematically analysed using SCAPS-1D to optimize device performance. The n-CdS/p- AgSbSe_2 single-junction optoelectronic device attains a PCE of 23.46%, with a J_{SC} of 44.42 mA cm^{-2} , a V_{OC} of 0.63 V, and an FF of 83.38%. With the integration of the various BSF layers, n-CdS/p- AgSbSe_2 /p⁺- $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ achieves the best photovoltaic performance among all studied structures, reaching an outstanding PCE of 34.32%, V_{OC} of 0.85 V, J_{SC} of 46.35 mA cm^{-2} , and an FF of 86.64%. Additionally, a peak responsivity of 0.819 A W^{-1} and detectivity of 2.93×10^{15} Jones are observed at 1100 nm for n-CdS/p- AgSbSe_2 /p⁺- $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ heterostructure, confirming its superior photodetection capability. The incorporation of the $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ BSF layer enriches the built-in potential from 0.94 to 2.37 V and boosts V_{OC} , enhancing PCE and detectivity. The superior band alignment between p- AgSbSe_2 and p⁺- $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ hetero-interface handles augmenting V_{OC} . This research identifies n-CdS/p- AgSbSe_2 /p⁺- $\text{Al}_{0.8}\text{Ga}_{0.2}\text{Sb}$ configuration as a viable and efficient solar cell and photodetector, offering high efficiency, long-term stability, and strong potential for real-world applications.

Conflicts of interest

None of the authors have any competing financial interests.

Data availability

Data will be available from the corresponding author upon reasonable request.

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