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# Computational study of a novel combination of dual-absorber structured perovskite solar cell with theoretical efficiency of 36.37%

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This research explores an innovative dual-absorber solar cell design that incorporates MAGel<sub>3</sub> and CsSnl<sub>3</sub> layers, aiming to achieve efficiency levels that exceed those of current single-junction solar cells. Simulations conducted with SCAPS-1D software identified optimal layer thicknesses for both materials, resulting in a maximum efficiency that significantly surpasses previously documented values for similar configurations. When considering defect densities, the optimized parameters revealed a strong open-circuit voltage, a high short-circuit current density, and an impressive fill factor, leading to a noteworthy overall efficiency even at certain defect levels. The enhanced performance of this dual-absorber design is attributed to the complementary bandgaps of the materials, which improve light absorption and charge carrier dynamics. Specifically, the smaller bandgap of  $CsSnI_3$  allows for more effective harvesting of lower-energy photons, and the higher bandgap of MAGel<sub>3</sub> helps in the absorption of higher-energy photons, while the dual-layer structure minimizes recombination losses. Further analyses of quantum efficiency and current-voltage characteristics support the architecture's potential to approach theoretical efficiency limits. This study suggests that the proposed dual-absorber configuration holds considerable promise for advancing solar cell technology and warrants further experimental validation.

### KEYWORDS

lead-free perovskite, dual absorber,  $CsSnI_3$ , MAGeI<sub>3</sub>, SCAPS 1D simulation, maximum photon absorption, bandgap management

# **1** Introduction

In recent years, thin-film solar cells have garnered substantial research interest due to improvements in efficiency and cost-effective manufacturing methods, making them ideal for diverse applications such as thermal energy and photovoltaic systems (Omid and Cora, 2020; Salve, 2020; Maoucha et al., 2023). Their advantages over traditional waferbased technologies include reduced material consumption and lower production costs. Growing efforts are directed at discovering novel materials to improve the efficiency-to-cost ratio. Lead-based perovskites, in particular, have exhibited exceptional optical and electrical properties, including a high absorption coefficient, low exciton binding energy, tunable bandgap, long diffusion lengths, and high carrier mobility, all achievable through low-cost fabrication (Roy et al., 2022; Teixeira et al., 2022). Thin-film solar cells can be manufactured via high-throughput and energy-efficient deposition techniques such as sputtering and chemical vapor deposition, which are better suited to scale than those used in silicon wafer technologies. Valeti et al. (2024) emphasized optimizing these processes for cost-effectiveness. Lead-based perovskite solar cells have reached conversion efficiencies of up to 26.7% (NREL, 2025; Interactive Best Research-Cell Efficiency Chart Photovoltaic Research, 2025), but they face major challenges like degradation and toxicity. Kamat et al. (2017) highlighted the urgency of solving stability and toxicity issues to make lead-free alternatives viable.

To overcome these limitations, researchers are turning to lead-free perovskites such as cesium germanium halides, which offer advantages like bandgap tunability, strong optical absorption, and improved conductivity (Dureja et al., 2022). Dureja et al. (2022) used SCAPS-1D simulations to design a Cs<sub>2</sub>SnI<sub>6</sub>-based solar cell, achieving 19.9% efficiency. Similarly, materials like MAGeI<sub>3</sub> (CH<sub>3</sub>NH<sub>3</sub>GeI<sub>3</sub>) and CsSnGeI<sub>3</sub> are gaining traction due to their high absorption in the visible-infrared range and greater stability than MAPbI<sub>3</sub> (Nalianya et al., 2021; Jan and Noman, 2023; Moone and Sharifi, 2024). Hybrid germanium-based perovskites show comparable photovoltaic performance to lead- and tinbased counterparts (Kumari et al., 2024) and have been studied with various electron transport layers (ETLs) and hole transport layers (HTLs) for optimal PCE (Panjikaran et al., 2024). To further boost efficiency, dual-absorber structures were introduced, stacking materials with different bandgaps to absorb a broader solar spectrum and reduce energy losses (Hemalatha et al., 2023). Bhattarai et al. (2023) simulated an MASnI<sub>3</sub>/CsSnGeI<sub>3</sub> dualabsorber design, achieving 31.53% efficiency by optimizing absorber thicknesses. Maoucha et al. (2023) combined MASnI<sub>3</sub> and CsSnGeI<sub>3</sub> with  $\mathrm{TiO}_2$  and Spiro-OMeTAD as transport layers to achieve 24.57% efficiency with a J<sub>SC</sub> of 28.11 mA/cm<sup>2</sup>, a VOC of 1.32 V, and a fill factor of 90.37%.

AlZoubi et al. (2023) studied MAGeI<sub>3</sub> cells with ZnOS and PEDOT-WO<sub>3</sub> transport layers, reaching nearly 16% efficiency. Jan and Noman (2023) explored planar and inverted structures of MAGeI<sub>3</sub> using SCAPS-1D and concluded that the inverted structure, especially with SnO<sub>2</sub> as the ETL and CuAlO<sub>2</sub> as the HTL, yielded a PCE of 25.43%, a VOC of 1.77 V, a J<sub>SC</sub> of 16.18 mA/cm<sup>2</sup>, and an FF of 89.02%. Focusing on CsSnI<sub>3</sub>, Ravidas et al. (2023) emphasized its potential due to a 1.3 eV bandgap, strong absorption, and high mobility. Their SCAPS-1D and DFT simulations showed superior performance with HTLs like Spiro-OMeTAD and CuI. Hossain et al. (2023a) and Hossain et al. (2023b) investigated over 70 architectures using CsSnI<sub>3</sub> and various ETLs (e.g., IGZO, WS<sub>2</sub>, TiO<sub>2</sub>, and C<sub>60</sub>), identifying ITO/ETL/CsSnI<sub>3</sub>/CuI/Au as the most promising.

The dual-absorber design marks a pivotal step forward in perovskite solar cell (PSC) development by expanding the absorption range and boosting PCE. Innovations like  $Ca_3NCl_3/Ca_3SbI_3$  absorbers further exemplify this progress, achieving improved VOC,  $J_{SC}$ , FF, and overall efficiency, which was approximately 30.22%, compared to individual absorber simulation (Ghosh et al., 2024; 2025).

Despite these benefits, insufficient transport layers can result in significant degradation due to energy and lattice mismatches. Consequently, innovative design strategies are crucial to address



Workflow of dual architecture simulation through SCAPS-1D.



these issues and improve the performance of lead-free perovskite solar cells. This study introduces an innovative lead-free perovskite solar cell design featuring a dual-absorber architecture composed of methylammonium germanium iodide (MAGeI<sub>3</sub>) and cesium tin iodide (Cs<sub>2</sub>SnI<sub>3</sub>). The cell utilizes MAGeI<sub>3</sub> as the wide bandgap front absorber ( $Eg \approx 1.9 \text{ eV}$ ) (Jeon et al., 2021) and Cs<sub>2</sub>SnI<sub>3</sub> as the narrow bandgap rear absorber ( $Eg \approx 1.3 \text{ eV}$ ) (Jeon et al., 2021), allowing for complementary light absorption from the visible to near-infrared spectrum.



The direct stacking of these materials creates a novel heterojunction interface, marking a first in fully lead-free perovskite photovoltaics. This layered architecture is distinct from conventional single-absorber PSCs or tandem cells, as it simplifies fabrication while achieving efficiencies exceeding 36%, surpassing the Shockley-Queisser limit, in this work. Energy band alignment analysis reveals a small conduction band offset (+0.2 eV) and a favorable valence band offset (-0.4 eV), which facilitates efficient charge separation and extraction without requiring a buffer layer. This approach simplifies the device structure while promoting low toxicity and cost-effectiveness. Additionally, simulations provide insights into interfacial properties, carrier dynamics, and optimization parameters, underscoring the potential of this architecture as a sustainable alternative in photovoltaic technology. Figure 1 shows the workflow of the simulated dual absorber architecture using SCAPS-1D and also the working points.

# 2 Numerical model and design

Despite the promising properties of hybrid lead perovskite solar cells, they face significant challenges, primarily due to their susceptibility to degradation and the inherent toxicity of lead (Osman et al., 2021; Moone and Sharifi, 2024). To address these issues, researchers have shifted their focus toward non-lead perovskite materials, with cesium germanium halide perovskites emerging as promising alternatives. These materials have demonstrated favorable characteristics, including tunable bandgaps, enhanced optical absorption, and brilliant optical conductivity (Maoucha et al., 2023; Panjikaran et al., 2024). In this work, CsSnI<sub>3</sub> and MAGeI<sub>3</sub> have been utilized as a double absorber layer and explored various parameters that are reported further.

## 2.1 Materials

The triumphant development of non-lead perovskites such as  $MAGeI_3$  ( $CH_3NH_3GeI_3$ ) and  $CsSnI_3$  has paved the way for high-throughput thin-film solar cells (Hemalatha et al., 2023; Panjikaran et al., 2024). These materials exhibit compelling electrical, optical, and processing properties that rival or surpass those of their lead-based counterparts. Specifically, they offer advantages such as bandgap tunability, large carrier mobility, strong visible–infrared range absorption coefficients, and improved stability compared to MAPbI<sub>3</sub>.

# 2.2 Simulation

The Solar Cell Capacitance Simulator (SCAPS) is a widely recognized and utilized software environment for solar modeling research, developed by the Electronic and Information Systems Department at Ghent University in Belgium (Burgelman et al., 2025; Al-Hattab et al., 2022). This simulation tool employs fundamental equations, including electron and hole Poisson equations, continuity equations, and transport equations, to model the capture of sunlight and the subsequent generation, movement, and extraction of electron-hole pairs in solar devices.

One of SCAPS's key strengths is its flexibility, allowing researchers to design and simulate specific solar devices by manipulating a broad range of material properties. The simulation outputs are invaluable for assessing the impact of various factors on device performance and for gaining insights into crucial solar cell characteristics. These include material defect density, defect placement, recombination rates, and band gap alignment across different layers of the device (Burgelman et al., 2004; Burgelman et al., 2025).

The versatility of SCAPS makes it an essential tool in addressing a wide spectrum of fundamental questions in both materials science and device physics related to solar cell technology. By enabling detailed simulations and analyses, SCAPS contributes significantly to the advancement of solar cell research and development.

The behavior and characteristics of charge carriers within solar devices are fundamentally described by three key equations:

- a) The Poisson equation
- b) The Continuity equation
- c) The Transport equation

These three equations collectively form the mathematical foundation for understanding and modeling the movement, distribution, and interactions of electrons and holes in solar cell structures. They provide a comprehensive framework for analyzing the electrostatic potential, charge carrier dynamics, and current flow within photovoltaic devices.

Fundamental equations used in the SCAPS-1D simulation software for modelling solar cell devices include

a) *Carrier Continuity Equation*: This equation describes the change in hole and electron concentrations over time, considering current densities, recombination, and generation processes (Islam et al., 2021).

$$\frac{dp}{dt} = -\left(\frac{1}{q}\right)\left(\nabla J_p\right) - R(x) + G(x) \tag{1}$$

$$\frac{dn}{dt} = \left(\frac{1}{q}\right) (\nabla J_n) - \mathbf{R}(\mathbf{x}) + \mathbf{G}(\mathbf{x})$$
(2)

In Equations 1, 2,  $J_p$  and  $J_n$  are hole and electron current densities, respectively.

TABLE 1 Parameters of the proposed model measured under one sun illumination.

Parameters	FTO	ZnO	MAGel <sub>3</sub>	CsSnl <sub>3</sub>	P3HT
Thickness (nm)	300	500	400	1,000	50
Bandgap (eV)	3.50	3.30	1.90	1.30	1.85
Electron affinity	4.00	4.0	3.98	3.60	3.10
Dielectric permittivity	9.00	9.0	10.0	28.0	3.40
Effective density of states (DOS) at the conduction band (CB) (cm <sup>-3</sup> )	2.20E18	2.2E18	1.00E16	1.57E19	1.00E22
Effective DOS at the valence band (VB) (cm <sup>-3</sup> )	1.80E18	1.9E19	1.00E15	1.47E18	1.00E22
Electron thermal velocity (m/s)	1.00E7	1.00E7	1.00E7	1.00E7	1.00E7
Hole thermal velocity (m/s)	1.00E7	1.00E7	1.00E7	1.00E7	1.00E7
Electron mobility (cm <sup>2</sup> /V.s)	2.00E1	1.00E2	1.62E2	5.00E1	1.00E-4
Hole mobility(cm <sup>2</sup> /V.s)	1.00E1	2.50E1	1.010E2	5.85E2	1.00E-3
Shallow uniform donor density $(N_D)$ (cm <sup>-3</sup> )	2.00E19	1.00E18	1.00E9	0	0
Shallow uniform acceptor density $(N_A)$ (cm <sup>-3</sup> )	0	0	1.00E9	1.00E17	3.170E13

R(x) and G(x) are recombination and generation processes, respectively.

b) *Diffusion–Drift Equations*: These equations describe the current densities for holes and electrons in terms of carrier concentrations, mobilities, and diffusion constants.

$$J_p = qn\mu_p - \frac{d\nu(x)}{dx} + qD_p\frac{dn}{dx}$$
(3)

$$J_n = qn\mu_n - \frac{d\nu(x)}{dx} + qD_n\frac{dn}{dx}$$
(4)

In the above Equations 3, 4,  $\mu_n$  and  $\mu_p$  are electron and hole mobilities and  $D_p$  and  $D_n$  are hole and electron diffusion constants, respectively.

c) *Poisson Equation*: This equation relates the electrostatic potential to charge carrier concentrations and doping densities in the semiconductor.

$$\nabla^2 V(x) = \frac{q}{s} \left[ p(x) - n(x) + N_D^+ - N_A^- \right]$$
(5)

Poisson equation is given in the Equation 5, where V(x) is the electrostatic potential,  $\varepsilon$  is the absorber permittivity, q is the electronic charge,  $N_D^+$  and  $N_A^-$  are the donor and acceptor densities, respectively, and finally, p(x) and n(x) are the position-dependent hole and electron concentrations.

**3 Device structure** 

The solar cell device structure investigated in this study comprises multiple layers, each serving a specific function to optimize the overall performance. Figure 2 shows the model of the proposed structure. The front electrode is composed of aluminum (Al), which provides a robust and conductive surface for electron collection. Beneath the Al layer, fluorine-doped tin oxide (FTO) is employed as the window layer due to its excellent transparency and conductivity, allowing maximum light penetration while facilitating electron transport. The electron transport layer (ETL) is made of zinc oxide (ZnO), which efficiently transports electrons from the perovskite absorber layers to the FTO.

The core of the device consists of two perovskite materials: methylammonium germanium iodide (MAGeI<sub>3</sub>) and cesium tin iodide (CsSnI<sub>3</sub>). These materials are strategically combined to enhance light absorption across a broader spectrum, leveraging their complementary bandgaps. This combination not only improves the absorption efficiency but also aids in defect passivation and charge carrier mobility. The hole transport layer (HTL) is composed of poly (3-hexylthiophene) (P3HT), which effectively transports holes to the back electrode. Finally, silver (Ag) is used as the back electrode, providing a high work function contact for efficient hole collection.

The integration of CsSnI<sub>3</sub> and MAGeI<sub>3</sub> within the device structure is particularly noteworthy. These perovskite materials exhibit high absorption coefficients and good charge carrier mobility, which are crucial for efficient photovoltaic performance. Their bandgap alignment facilitates a graded bandgap structure, driving charge carriers toward their respective electrodes and reducing recombination losses. This innovative combination aims to leverage the strengths of both materials, resulting in a more efficient and stable solar cell.

## 3.1 Working mechanism

The working mechanism of the proposed device is shown in Figure 3. When photons with energy greater than



#### FIGURE 4

(A) Change in  $V_{OC}$  with respect to the variation in CsSnl<sub>3</sub> thickness; (B) change in  $J_{SC}$  with respect to the variation in CsSnl<sub>3</sub> thickness; (C) change in fill factor with respect to the change in CsSnl<sub>3</sub> thickness; (D) change in efficiency with respect to the thickness change in CsSnl<sub>3</sub>.

P3HT Thickness (µm)	V <sub>OC</sub> (V)	J <sub>sc</sub> (mA/cm²)	FF (%)	Efficiency (%)
0.01	1.1736	34.7876	77.51	31.65
0.02	1.1716	34.7878	75.45	30.75
0.05	1.1655	34.7877	70.61	28.63
0.1	1.1549	34.7877	59.59	23.94

### TABLE 2 Variation of P3HT thickness.

or equal to the band gap of the absorber layers (MAGeI<sub>3</sub> and CsSnI<sub>3</sub>) fall on the solar cell, they excite electrons from the valence band to the conduction band, creating electron-hole pairs. In the MAGeI<sub>3</sub> layer, photons with energy greater than 1.78 eV excite electrons from the valence band (-5.7 eV) to the conduction band (-3.92 eV). These excited electrons then move through the MAGeI<sub>3</sub>

layer to the ZnO layer. Similarly, in the CsSnI<sub>3</sub> layer, photons with energy greater than 1.4 eV excite electrons from the valence band (-5.0 eV) to the conduction band (-3.6 eV). The electrons in the conduction band of CsSnI<sub>3</sub> move toward the ZnO layer, while the holes left in the valence band of CsSnI<sub>3</sub> move toward the P3HT layer.



The electrons that reach the ZnO layer are collected by the FTO layer and then move toward the Al electrode, while the holes that reach the P3HT layer are collected by the Ag electrode. This movement of electrons and holes ensures efficient charge separation and collection, converting light into electrical energy. The energy band diagram helps visualize this process by showing the energy levels and the direction of electron and hole movement, with curved arrows indicating the pathways for electrons and holes. This mechanism utilizes the different band gaps of the absorber layers to capture a broader spectrum of sunlight, enhancing the efficiency of the solar cell.

# 4 Results and discussion

The input property values of the proposed model are given below in Table 1. These are the optimized values received for the maximum efficiency generating device with and without consideration of the defect densities.

# 4.1 Effect of CsSnl<sub>3</sub> and MAGel<sub>3</sub> thickness changes

The thicknesses of the absorber layers of CsSnI<sub>3</sub> and MAGeI<sub>3</sub> were varied and plotted, and the effects of changing the thicknesses were investigated. The opto-electronic characteristics were studied under the AM1.5 illumination. The plots presented in Figures 4A–D illustrate the behavioral patterns of open-circuit voltage ( $V_{OC}$ ), short-circuit current density ( $J_{SC}$ ), fill factor, and efficiency as the thickness of the CsSnI<sub>3</sub> layer is varied from 200 nm to 1,000 nm. It is observed that with an increase in the thickness of the CsSnI<sub>3</sub> layer, both  $V_{OC}$  and fill factor exhibit a slight decreasing trend, while the current and efficiency curves show an upward trend. This might be because of the band alignment mismatch, due to which interfacial recombination can occur. The optimal results are achieved with a CsSnI<sub>3</sub> thickness of 1,000 nm, yielding values of  $V_{OC} = 1.23$  V,  $J_{SC}$ 

= 34.79 A, a fill factor of 84.35%, and an efficiency of 36.37%, which represent the highest values recorded to date. On the other hand, no significant changes were seen when we varied the thickness of the  $MAGeI_3$  layer.

### 4.2 Effects of variation in P3HT thickness

In this proposed model, the hole transport layer P3HT thickness is varied from 0.01  $\mu$ m to 0.1  $\mu$ m, and the results are given in Table 2. It is observed that the optimum performance of the device is achieved at the P3HT layer thickness of 0.01  $\mu$ m. In the experimental aspect, acquiring a thickness of 10 nm is impractical, so the HTL thickness is fixed at 50 nm.

# 4.3 Effects of defect density in the $CsSnl_3$ and MAGel<sub>3</sub> layers

Figure 5 shows the difference in the device performance with and without the defects. We investigated the incorporation of defect levels in CsSnI<sub>3</sub> and MAGeI<sub>3</sub> layers, ranging from  $1 \times 10^{10}$  to  $1 \times 10^{14}$ , and analyzed their impact on open-circuit voltage (V<sub>OC</sub>), short-circuit current density (J<sub>SC</sub>), fill factor, and overall device efficiency. The resulting graphs are shown in Figures 6A–D. The observed trend indicates that both V<sub>OC</sub> and J<sub>SC</sub> remain relatively stable up to a defect concentration of  $1 \times 10^{12}$ , after which a decline is noted. Conversely, the fill factor exhibits a decreasing trend with increasing defect levels up to  $1 \times 10^{12}$ , followed by a slight improvement. When we also consider the MAGeI<sub>3</sub> layer, the device efficiency also decreases, as anticipated in the presence of defects. Consequently, we determine the optimal defect level to be  $1 \times 10^{12}$ .

# 4.4 Effects of temperature variation on the proposed device

The density of states in the conduction and valence bands varies with temperature, as follows in the Equations 6–8, where  $T_0$  represents the default temperature, set at 300 K, where the parameter value should be defined in SCAPS-1D. Similarly, the thermal velocity ( $V_{th}$ ) is also influenced by temperature, as shown in the following equations. All other parameters are considered to be independent of temperature. The diffusion coefficient used in the calculations, given by  $D = \mu KT$ , is temperature-dependent, which contradicts the information provided in the initial SCAPS manual.

$$N_{\rm C}(T) = N_{\rm C}(T_0) \left\{ \frac{T}{T_0} \right\}^{1.5}$$
 (6)

$$N_{V}(T) = N_{V}(T_{0}) \left\{ \frac{T}{T_{0}} \right\}^{1.5}$$
 (7)

$$V_{\rm th}(T) = V_{\rm th}(T_0) \left\{ \frac{T}{T_0} \right\}^{0.5}$$
 (8)

Figure 7 shows J–V (current density vs. voltage) curves for different temperatures, each represented by a distinct color and symbol. As temperature increases, we observe a slight shift in the curves, indicating changes in the device's electrical characteristics.

Temperature	V <sub>OC</sub> (V)	J <sub>SC</sub> (mA/cm²)	Fill Factor (%)	Efficiency (%)
260	1.2047	34.7864	72.7574	30.491
280	1.1879	34.7871	71.5468	29.5669
300	1.1654	34.7877	70.6053	28.6262
320	1.1318	34.7884	70.2899	27.6774
340	1.0878	34.7892	70.6215	26.7275
360	1.0378	34.7898	71.3124	25.748
380	0.9852	34.7901	72.1003	24.7138

TABLE 3 Solar parameters with respect to temperature variation.



The open-circuit voltage (V<sub>OC</sub>) appears to decrease slightly with increasing temperature, which is typical for solar cells due to increased carrier recombination at higher temperatures. However, the short-circuit current density (J<sub>sc</sub>) seems to increase with

temperature, likely due to enhanced carrier generation. The overall shape of the curves suggests that the fill factor may also be affected by temperature changes, potentially improving slightly at higher temperatures. These temperature-dependent variations in



TABLE 4 Device parameters with varied dopant concentrations.

N <sub>A</sub> (cm <sup>-3</sup> )	$1 \times 10^{14}$	$1 \times 10^{15}$	$1 \times 10^{16}$	$1 \times 10^{17}$
V <sub>OC</sub> (V)	1.1652	1.1652	1.1652	1.1655
J <sub>SC</sub> (mA/cm <sup>2</sup> )	34.7935	34.7915	34.7892	34.7877
FF (%)	68.48	68.48	68.55	70.61
Efficiency (%)	27.76	27.76	27.79	28.63

Bold values indicate optimized values.

TABLE 5 Device performance while varying  $R_S,$  when  $R_{SH}$  is fixed at  $10^{30}\,\Omega\text{-}\text{cm}^2.$ 

R <sub>S</sub> (Ω)	V <sub>oc</sub> (V)	J <sub>sc</sub> (mA/cm²)	FF (%)	Efficiency (%)
0	1.1655	34.7877	70.61	28.63
2	1.1655	34.7875	65.13	26.41
4	1.1655	34.7873	59.77	24.23
6	1.1655	34.7872	54.55	22.12
8	1.1656	34.7870	49.60	20.11
10	1.1656	34.7868	44.88	18.20

Bold values indicate optimized values.

 $V_{\rm OC}, J_{\rm SC},$  and fill factor collectively influence the device's efficiency, with the optimal operating temperature likely falling within the measured range. Table 3 shows the values of the parameters.

We also investigated the effects of temperature variation on the device, systematically varying the temperature

TABLE 6	Device performance	while varying	R <sub>SH</sub> , when	R <sub>s</sub> is fixed	l at 0.5 $\Omega$
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R <sub>SH</sub> (Ω)	V <sub>oc</sub> (V)	J <sub>sc</sub> (mA/cm²)	FF (%)	Efficiency (%)
10	0.3479	33.1311	25.01	2.88
10 <sup>2</sup>	1.0323	34.6146	59.21	21.16
10 <sup>3</sup>	1.1202	34.7702	70.25	27.36
10 <sup>4</sup>	1.1572	34.7859	69.55	28.00
10 <sup>5</sup>	1.1646	34.7875	69.27	28.06
10 <sup>6</sup>	1.1654	34.7876	69.23	28.07
10 <sup>8</sup>	1.1655	34.7877	69.23	28.07
10 <sup>10</sup>	1.1655	34.7877	69.23	28.07

Bold values indicate optimized values.

from 260 K to 380 K. Figure 7 illustrates the impact of temperature changes on open-circuit voltage ( $V_{OC}$ ), short-circuit current density ( $J_{SC}$ ), fill factor, and device efficiency. It is observed that  $V_{OC}$  exhibits a slight decrease, while  $J_{SC}$  increases with rising temperature. This behavior can be attributed to changes in carrier mobility as the temperature increases. The fill factor decreases until approximately 320 K, after which it begins to rise. In contrast, device efficiency decreases linearly with increasing temperature. This pattern is evident in Figures 8A–D.

### 4.5 Effect of dopant concentration

In the proposed device, when the dopant concentration of the CsSnI<sub>3</sub> absorber layer was varied from  $1 \times 10^{14}$  to  $1 \times 10^{17}$ , it was observed, from Table 4, that solar parameters values increased, especially Voc, device efficiency and fill factor, giving the maximum efficiency of 28.63%, with a fill factor of 70.61% and a V<sub>OC</sub> of 1.1655 V. J<sub>SC</sub>, on the other hand, was seen declining, possibly because of the chance of recombination rate due to the increase in the carriers. No particular changes were seen in the parameters when we changed the dopant concentration in the layer of MAGeI<sub>3</sub>.

## 4.6 Effects of parasitic resistances

Series and shunt resistances are critical parameters in solar cells affecting their efficiency. The former is due to the current movement through the cell's emitter and base as well as contact resistances. High series resistance reduces the fill factor and J<sub>SC</sub>, impacting the overall performance of the device.

On the other hand, shunt resistance arises due to manufacturing defects. If the shunt resistance is low, it can create alternate current paths, reducing voltage and current flow, particularly under low light conditions, resulting in significant power losses. Ideally, it is



desired that the series resistance should be minimum, and the shunt resistance should be maximum.

### 4.6.1 Effect of series resistance

In this proposed model, the series resistance was varied from 0  $\Omega$  to 10  $\Omega$ , respectively, by fixing  $R_{SH}$  at  $10^{30}~\Omega\text{-cm}^2$ . Table 5 gives the respective values of solar parameters. The pattern observed is that an increase in series resistance affects  $J_{SC}$  and fill factor, thus affecting the overall efficiency.

### 4.6.2 Effect of shunt resistance

In this proposed model, shunt resistance  $(R_{SH})$  is varied from 10  $\Omega$ -cm<sup>2</sup> to  $10^{10}$   $\Omega$ -cm<sup>2</sup>, respectively, by fixing series resistance  $(R_S)$  at 0.5  $\Omega$ . Table 6 gives the values of solar parameters with respect to shunt resistance change. The pattern observed is that, as shunt resistance increases, each parameter improves, and thus the overall performance of the device also improves. Table 6 shows the pattern.

### 4.7 Effect of quantum efficiency

Quantum efficiency in solar cells measures how efficiently incident photons are converted into electric current. It is typically expressed as a combination of external quantum efficiency (EQE) and internal quantum efficiency (IQE). The former is attributed to optical losses, and the latter reflects the efficiency of charge carrier collection from absorbed photons. Different absorber layers significantly impact quantum efficiency (QE). The choice of materials affects absorption characteristics and recombination rates, influencing overall efficiency.

Replacing a single layer of MAGeI<sub>3</sub> with double layers of MAGeI<sub>3</sub> and  $CsSnI_3$  can enhance the quantum efficiency of solar devices. This configuration benefits from the complementary bandgaps, improving light absorption and charge carrier dynamics.

CsSnI<sub>3</sub>, with its smaller bandgap, allows for better harvesting of lower-energy photons, potentially increasing overall efficiency beyond that of MAGeI<sub>3</sub> alone. The combination can also reduce recombination losses, further boosting performance. Figure 9 shows



TABLE 7 Optimized structure parameters before and after adding defect density  $N_t = 1 \times 10^{12}$ .

Solar parameters	Optimized structure without defects	Optimized structure with defects
V <sub>OC</sub> (V)	1.2872	1.1736
J <sub>SC</sub> (mA/cm <sup>2</sup> )	34.791	34.787
Fill factor (%)	87.50	77.51
Efficiency (%)	36.37	27.78

the comparison of the two devices, one with a single junction of  $MAGeI_3$  and one device with dual-absorber layers of  $MAGeI_3$  and  $CsSnI_3$ . The latter shows a better result, promising good practical output.

# 5 Conclusion

In this study, two absorber layers, specifically MAGeI<sub>3</sub> and CsSnI<sub>3</sub>, were utilized as a dual-absorber configuration. Simulations conducted using SCAPS-1D software indicated that the optimal thickness for MAGeI<sub>3</sub> is 0.4 µm, while for CsSnI<sub>3</sub>, it is 1.0 µm, achieving a maximum efficiency of 36.37% under defect-free conditions, the highest reported to date. Further investigations incorporating defect densities in each layer and also interfacial defect densities revealed optimal solar parameters of Voc = 1.1475 V, Jsc = 34.79 mA/cm<sup>2</sup>, FF = 69.61%, and efficiency = 27.78% at a defect density of  $1 \times 10^{12}$  cm<sup>-3</sup> and interfacial defect of  $1 \times 10^{10}$  cm<sup>-3</sup> (P3HT/CsSnI<sub>3</sub>; CsSnI<sub>3</sub>/MAGeI<sub>3</sub>; MAGeI<sub>3</sub>/ZnO). Temperature analysis demonstrated that 300 K is ideal for maximizing output in this architecture. Additionally, quantum efficiency (QE) and current-voltage (JV) analyses were conducted, highlighting the efficacy of the proposed

novel architecture in approaching the Shockley–Queisser limit, warranting further experimental exploration, as this configuration has yet to be synthesized. Table 7 shows the results with and without optimization of device architecture.

Discussion is warranted in bringing this configuration to the experimental set-up because this architecture is to be constructed through sequential deposition, which can pose stability issues and interfacial defects. This can be another bottleneck to be overcome and is a problem worthy of further attention.

# Data availability statement

The datasets presented in this study can be found in online repositories. The names of the repository/repositories and accession number(s) can be found in the Supplementary Material.

# Author contributions

VG: formal analysis, investigation, methodology, software, writing - original draft, and writing - review and editing.

SP: conceptualization, formal analysis, methodology, software, supervision, writing – original draft, and writing – review and editing.

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# Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships

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that could be construed as a potential conflict of interest.

# **Generative AI statement**

The author(s) declare that no Generative AI was used in the creation of this manuscript.

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# Supplementary material

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fenrg.2025. 1631201/full#supplementary-material

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