

# Numerical Simulation Analysis of Two-Terminal Monolithic Perovskite-CIGS Tandem Solar Cell for Enhanced Photovoltaic Performance Using SCAPS-1d

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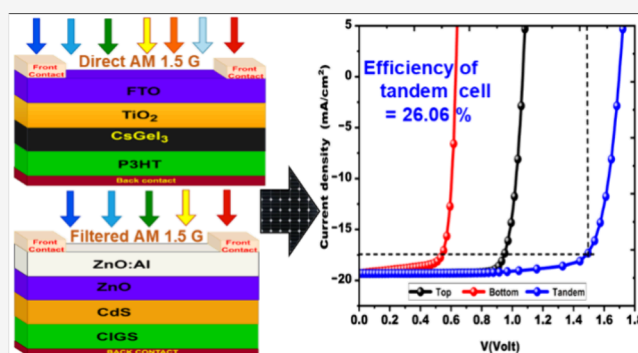
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**ABSTRACT:** This research designs and simulates a high-efficiency tandem solar cell (TSC) using SCAPS-1D (3.3.12), exploiting tandem perovskite technology for enhanced performance. The agenda of our work is here to minimize the two largest losses associated with single-junction solar cells like thermalization and transmission losses by absorbing a broader spectrum of sunlight using CsGeI<sub>3</sub>/CIGS tandem solar cell technology. To ensure the accuracy of the simulated results, the authors first calibrate both the top and bottom solar cells using experimental data and compare the simulated results with experimental findings. This study investigates the impact of thickness, parasitic resistance, temperature, quantum efficiency, band diagram, absorption coefficients, and two-diode model equivalent circuit parameters on solar cell performance. This work optimizes lead-free, wide bandgap (1.6 eV) CsGeI<sub>3</sub> perovskite and narrow bandgap (1.1 eV) CIGS solar cells individually and then proposes a tandem solar cell structure using a filtered spectrum approach. The proposed CsGeI<sub>3</sub>/CIGS tandem solar cell device structure is studied in detail and simulated using SCAPS 1D. A tandem configuration, with a thickness of a 273 nm top cell (simulated under AM1.5G) and a 1000 nm bottom cell, achieved conversion efficiencies of 16.93% and 16.49%, respectively, with respective  $J_{SC}$  values of 19.31 mA cm<sup>-2</sup>/19.32 mA cm<sup>-2</sup>. By adding the voltages at same current points to make the tandem J-V curve, this design yielded a 26.06% efficient perovskite-CIGS tandem cell with  $V_{OC}$  of 1.73 V,  $J_{SC}$  of 19.32 mA cm<sup>-2</sup>, and FF of 77.98%. This perovskite-CIGS tandem design demonstrates a promising route for developing high-efficiency, low-cost TSCs.



## 1. INTRODUCTION

Perovskite-based tandem solar cells hold promise as a cost-effective photovoltaic technology due to their potential for high power conversion efficiency (PCE) through the optimized utilization of the solar spectrum.<sup>1</sup> Silicon, CIGS, and low-bandgap perovskite are promising bottom cell materials for efficient tandem solar cells to meet increasing energy demands.<sup>2</sup> The world faces a significant challenge in meeting growing energy demands.<sup>3</sup> Global energy consumption is projected to rise from 472 Quads in 2006 to 678 Quads in 2030, representing an average annual increase of 1.8%.<sup>4</sup> Harvesting just 0.02% of solar energy reaching earth would meet our energy needs.<sup>5</sup> Currently, the energy requirement is mainly fulfilled by fossil fuels followed by renewable sources of energy such as wind, hydro, and solar.<sup>6</sup> Solar power offers a promising avenue for safe and sustainable energy, and tandem solar cells can help overcome the efficiency limitations of photovoltaic modules.<sup>1</sup> Researchers are extensively investigating semiconductor materials to develop efficient, cost-effective, and long-lasting solar cells (SCs). Currently, various single-

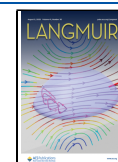
junction c-Si cells<sup>7,8</sup> command over 90% of global solar production. Silicon solar cells exceed 26% power conversion efficiency.<sup>9</sup> Silicon solar cells, while dominant, suffer from complex fabrication, rigidity, limited light absorption, and poor flexibility (<30 degrees), driving the search for alternative materials and suggested designs to enhance performance and sustainability. Single-junction (1N) SCs are limited to a maximum efficiency of 33% according to the Shockley and Quessier (S-Q) limit.<sup>10</sup> A pictorial representation of lattice thermalization losses and nonabsorbed photon losses is shown in Figure 1a, and these losses are the primary reasons not to conquer the SQ limit by single-junction solar cells.<sup>11</sup> To minimize these losses and efficiently utilize the maximum

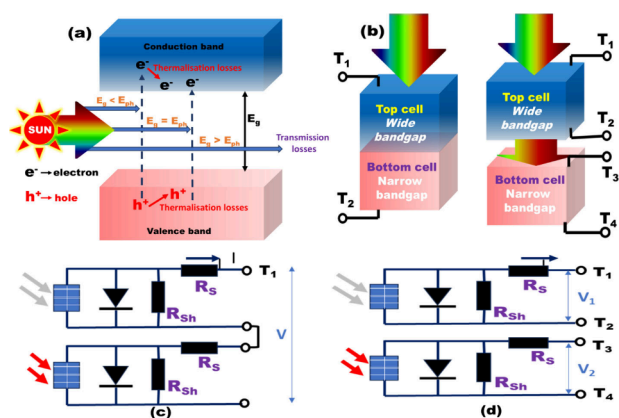
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**Figure 1.** (a) Power loss diagram for single-junction solar cells, including thermalization and transmission losses; (b) 2-T (left) and 4-T (right) architectures for perovskite/CIGS tandem solar cells; (c) Equivalent circuit of 2-T tandem cell; (d) Equivalent circuit of 4-T tandem cell.

spectrum, both wide and narrow bandgap materials are utilized for designing top and bottom solar cells that open the door for tandem solar cell technology; this idea was presented by Jackson in 1955.<sup>12</sup> Tandem cells were designed by using wide bandgap top cells (1.5–1.9 eV) and narrow bandgap bottom cells (0.9–1.3 eV) to absorb a wider range of the light spectrum. This design allows effective absorption of high-energy photons by the top cell, diminishing thermalization losses and producing a high voltage. Concurrently, the bottom cell traps low-energy photons shown in Figure 1b that penetrate through improving the overall utilization of the solar spectrum.<sup>13</sup> The two most common tandem architectures are mechanically stacked four-terminal (4 T) tandem and two-terminal (2 T) monolithic structures, as shown in Figure 1b, and equivalent circuits of 2-T and 4-T perovskite/CIGS tandem solar cells shown in Figure 1c,d. The 2T monolithic structure connects solar cells in series by matching their current densities, minimizing power loss through interconnection layers and treating the device as a single unit. In 1980, Lamort et al. developed a series-connected dual-junction photovoltaic cell.<sup>14</sup> Kim et al. achieved a record 19.8% efficiency for CIGS/Si tandem cells.<sup>15</sup> Mousa et al. achieved 30.52% efficiency with  $\text{MaPbI}_3/\text{CIGS}$  tandem solar cells in 2021.<sup>16</sup> Top cells can utilize both inorganic and organic materials with a wide bandgap. Inorganic materials like CdTe, Si, CIGS, and GaAs are potential candidates that offer excellent mobility and absorption coefficient and exceptional radiation resistance.<sup>17</sup> Tandem architectures offer a promising route to improve solar cell efficiency, with several configurations like perovskite/silicon,<sup>18,19</sup> perovskite/CIGS,<sup>2,20</sup> and perovskite/perovskite<sup>21–25</sup> tandems along with all quantum dot solar cell structures.<sup>26,27</sup> Perovskites exhibit strong light absorption and simple solution-based fabrication, leading to rapid efficiency gains from 3.8% in 2009 to 25.70% in 2024.<sup>28</sup> Perovskites are well-suited for tandem solar cells due to their excellent photoelectric properties, tunable band gaps, mechanical durability, low cost, and solution-based fabrication.<sup>29</sup> Researchers have identified metal halide perovskites ( $\text{ABX}_3$ ), which absorb light in the visible spectrum, for potential application in photovoltaic technology, and later they are named after the Russian mineralogist L. A. Perovski. Cesium (Cs), methylammonium (MA), and formamidinium (FA) are

typically denoted as A (monovalent cation), with Pb or Sn as B (divalent cation), and I, Br, or Cl as X (halide anion). Perovskites are a strong candidate for photovoltaics due to their low cost, variable bandgap (1.1–2.3 eV), good carrier mobility ( $\mu_e \sim 5\text{--}10 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  and  $\mu_h \sim 1\text{--}5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ), and long carrier lifetime ( $\sim 1 \mu\text{s}$ ).<sup>30</sup> Perovskite tandem solar cells, first appearing in 2014 with approximately 14% conversion efficiency, have since achieved efficiencies exceeding 25% (Werner et al.), 23.6% (Bush et al.), and 25.2% (Sahli et al.).<sup>21</sup> Among these, perovskite/CIGS TSCs have demonstrated substantial compensations in bandgap tunability, versatility, and durability.<sup>31</sup> In this work, the authors focus on lead-free perovskite/CIGS tandem solar cells. CIGS is a well-established light absorber for PV cells due to its optimal bandgap, high absorption coefficient (up to  $10^7 \text{ m}^{-1}$ ), and excellent stability.<sup>32</sup> CIGS is highly suitable for designing tandem solar cells as it offers a tunable bandgap ranging from 1.04 to 1.69 eV by adjusting the gallium (Ga) content in the CIGS material.<sup>33</sup> In this work, after detailed investigations, lead-free  $\text{CsGeI}_3$  perovskite with a bandgap of 1.6 eV is found suitable for perovskite/CIGS tandem solar cell.<sup>34–42</sup> Its high absorption coefficient enables efficient light harvesting and enhanced carrier generation and transport. Chen et al. first fabricated lead-free  $\text{CsGeI}_3$  halide perovskite via a simple solvothermal route, achieving a power conversion efficiency of approximately 4.92% under an AM of 1.5 G after tuning the  $\text{CsGeI}_3$  quantum rod configuration.  $\text{CsGeI}_3$ , a lead-free and novel perovskite material, requires consideration of its environmental stability over long-term usage, particularly under high-temperature and high-humidity conditions. Krishnamoorthy et al.'s computational and experimental results on  $\text{CsGeI}_3$  suggest germanium as a suitable lead substitute in halide perovskites for solar cells. Their experimental photocurrent results of approximately  $5.7 \text{ mA/cm}^2$  confirm the durable potential of Ge-based lead-free halide perovskite compounds in photovoltaic applications.<sup>43</sup> CIGS, a mature thin-film material, is well-suited for solar cells due to its broad light absorption, efficient charge transport, and high stability. CIGS is a highly efficient thin-film semiconductor used in photovoltaics because of its direct bandgap and strong light absorption. The bandgap, tunable from 1.0 to 1.7 eV by adjusting the Ga/In ratio, optimizes spectral utilization for tandem applications. Low defect density and high carrier mobility ensure superior charge transport, boosting the power conversion efficiency. Interface engineering and doping strategies improve junction properties, minimizing recombination losses and enhancing stability. CIGS solar cells, achieving efficiencies over 23%, are a competitive alternative to silicon photovoltaics.<sup>44</sup> CIGS solar cells offer advantages over silicon due to their thin-film construction, resulting in lighter weight and greater flexibility. Furthermore, CIGS exhibits a lower temperature coefficient, maintaining higher efficiency in hot climates compared to silicon.<sup>45</sup> Perovskite and CIGS thin-film solar cells offer flexible, lightweight devices with high power-to-weight ratios, making them well-suited for space applications.<sup>46,47</sup> This study focuses on materials with a high technological potential and significant field impact. They were selected for their sustainability and promising manufacturability in next-generation photovoltaics. This study seeks a cost-effective and stable lead-free perovskite material to improve the efficiency of perovskite/CIGS tandem solar cells. All perovskite-CIGS TSCs are an emerging PV technology for high-efficiency SCs. The primary goal of this study is to

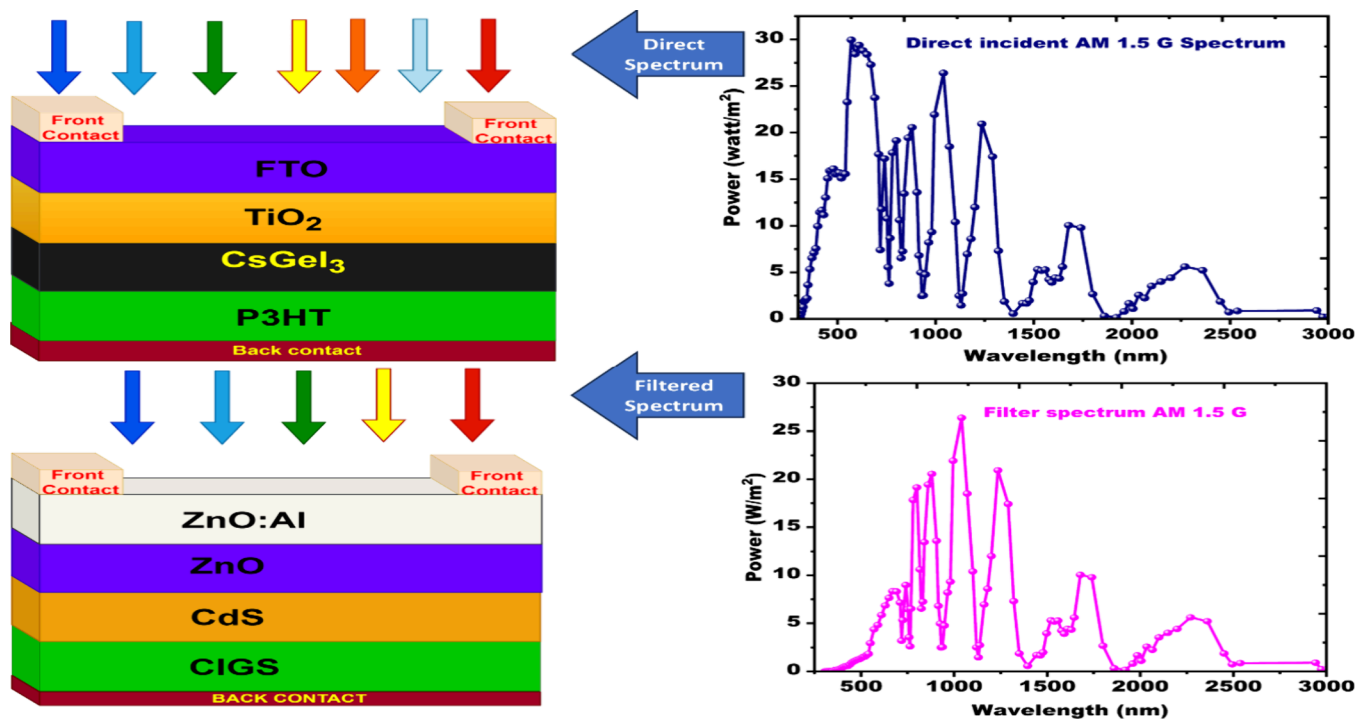


Figure 2. Tandem solar cell architectures using direct and filtered AM 1.5G spectrum.

optimize the device parameters of an environmentally friendly CsGeI<sub>3</sub>/CIGS tandem solar cell to maximize its performance, positioning it as a potential alternative to lead-based counterparts. This is achieved by tuning the thicknesses of the top and bottom cells to ensure current matching, thereby improving the overall efficiency by reducing thermalization and transmission losses typical in single-junction solar cells. Furthermore, the choice of a perovskite/CIGS tandem structure over the conventional perovskite/silicon tandem is primarily motivated by its lightweight nature and compatibility with flexible substrates. In existing research, lead (Pb), a hazardous substance, was employed in the top cells of perovskite solar cells.<sup>48</sup> Given lead's mutagenic toxicity and associated health risks, a lead-free tandem solar cell structure is proposed after detailed investigation.<sup>49</sup> The proposed perovskite/CIGS tandem solar cell offers a 26.06% conversion efficiency. Tandem cell research advances solar energy by increasing efficiency and exploring innovative materials and designs. These improvements lead to more cost-effective PV cells, reduce recombination, and accelerate the adoption of sustainable energy sources.

## 2. MATERIALS AND METHODS

Employing simulation and modeling in semiconductor device design saves time and resources by enabling researchers to validate theoretical computations prior to fabrication.<sup>50</sup> The CsGeI<sub>3</sub>/CIGS tandem solar cell simulation is conducted using SCAPS-1D, a widely used powerful tool among photovoltaic researchers worldwide that accommodates extensive variations in material input parameters, yielding realistic results closely aligned with experimental data.<sup>51–54</sup> The fundamental equations guiding this simulation are continuity (eq 1), current densities of electron and holes given by equations (eqs 2 and 3) and Poisson's equation (eq 8), along with some other supporting equations for free charge carriers given by the following equations.<sup>55</sup>

Continuity equations for an electron and holes:

$$\frac{\partial j_n}{\partial x} + G_n(x) - R_n(x) = 0 \quad \text{and} \quad \frac{\partial j_p}{\partial x} - G_p(x) + R_p(x) = 0 \quad (1)$$

The corresponding current densities of electron and holes are given by eqs 2 and 3.

$$J_n = q \left( D_n \frac{dn}{dx} + \mu_n n \frac{d\phi}{dx} \right) \quad (2)$$

$$J_p = -q \left( D_p \frac{dp}{dx} - \mu_p p \frac{d\phi}{dx} \right) \quad (3)$$

Diffusion length and diffusivity describe how far and how fast charge carriers (electrons and holes) move before recombining. They are given by an equation (eqs 4 and 5).

$$\text{Diffusion length: } L_{n,p} = \sqrt{D_{n,p} \tau_{n,p}} \quad (4)$$

$$\text{Diffusivity: } D_{n,p} = \left[ \left( \frac{k_B T}{q} \right) \mu_{n,p} \right] \quad (5)$$

The open-circuit voltage of the solar cell when no current is drawn is given by eq 6. The carrier lifetime, i.e., the average time of a photogenerated carrier existing before recombining, is given by eq 7.

$$\text{Open circuit voltage: } V_{OC} = \left( \frac{nk_B T}{e} \right) \left[ \ln \left( \frac{I_L}{I_0} + 1 \right) \right] \quad (6)$$

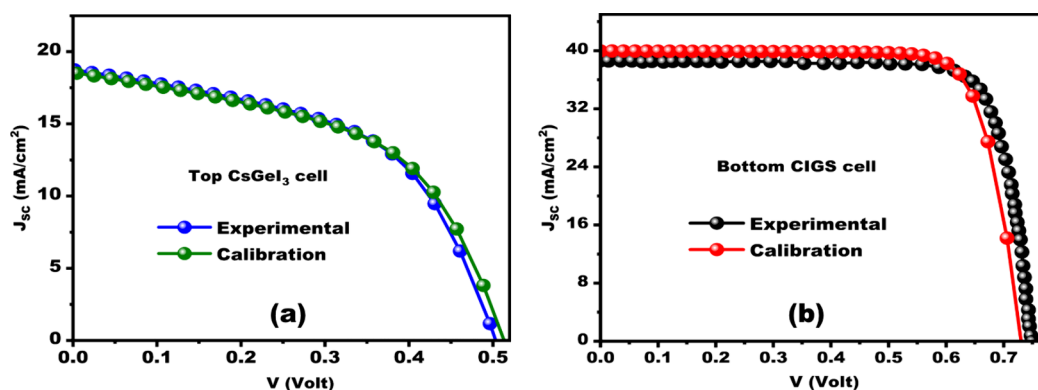
$$\text{Carrier lifetime: } \tau = \frac{1}{\sigma N_t V_{th}} \quad (7)$$

$$\begin{aligned} \text{Poisson's equation: } & \frac{d^2}{dx^2} V(x) \\ & = \frac{q}{\epsilon_0 \epsilon_r} [p(x) - n(x) + N_D - N_A + \rho_p - \rho_n] \end{aligned} \quad (8)$$

The electrostatic potential is  $V(x)$ , and the electron charge is  $q$ . Vacuum and relative permittivity are  $\epsilon_0$  and  $\epsilon_r$ , respectively. Donor and acceptor densities are  $N_D$  and  $N_A$ , while hole and electron

Table 1. SCAPS Input Parameter for Various Layers of Top and Bottom Solar Cells Adopted from the Literature<sup>35,56–58</sup>

Material Properties	Top cell				Bottom Cell			
	CsGeI <sub>3</sub>	P3HT	TiO <sub>2</sub>	FTO	CIGS	CdS	ZnO	ZnO:Al
Thickness (nm)	273	40	40	50	1000	45	50	100
Bandgap (eV)	1.6	2.0	3.2	3.5	1.1	2.4	3.3	3.6
Electron affinity (eV)	3.52	3.2	3.9	4.0	4.31	4.2	4.4	4.4
Dielectric permittivity ( $\epsilon_r$ )	18.0	4.2	9.0	9.0	13.6	10	9.0	9.0
CB effective DOS $N_C$ (cm <sup>-3</sup> )	$1.0 \times 10^{18}$	$2.0 \times 10^{21}$	$2.0 \times 10^{18}$	$2.0 \times 10^{18}$	$2.2 \times 10^{18}$	$2.2 \times 10^{18}$	$2.2 \times 10^{18}$	$1.0 \times 10^{18}$
VB effective DOS $N_V$ (cm <sup>-3</sup> )	$1.0 \times 10^{19}$	$2.0 \times 10^{21}$	$1.8 \times 10^{19}$	$1.8 \times 10^{19}$	$1.8 \times 10^{19}$	$1.8 \times 10^{19}$	$1.8 \times 10^{18}$	$1.0 \times 10^{19}$
Electron mobility $\mu_n$ (cm <sup>2</sup> V s <sup>-1</sup> )	20	$1.8 \times 10^{-3}$	100	20	100	100	100	100
Hole mobility $\mu_p$ (cm <sup>2</sup> V s <sup>-1</sup> )	20	$1.8 \times 10^{-3}$	25	10	25	25	25	30
Donor density, $N_D$ (cm <sup>-3</sup> )	0	0	$1.0 \times 10^{16}$	$1.0 \times 10^{15}$	0	$1.0 \times 10^{18}$	$1.0 \times 10^{18}$	$1.0 \times 10^{19}$
Acceptor Density $N_A$ (cm <sup>-3</sup> )	$2.0 \times 10^{16}$	$1.0 \times 10^{19}$	0	0	$9.0 \times 10^{16}$	0	0	0
$N_t$ (cm <sup>-3</sup> )	$1.0 \times 10^{15}$	$1.0 \times 10^{15}$	$1.0 \times 10^{15}$	$1.0 \times 10^{15}$	$1.0 \times 10^{14}$	$1.0 \times 10^{18}$	$1.0 \times 10^{17}$	$1.0 \times 10^{17}$
<b>Interfacial parameters</b>								
Interface	$N_t$ (cm <sup>-2</sup> )	Defect Energy level $E_t$ (eV)	Defect type	Capture Cross Section of electrons/holes (cm <sup>2</sup> )				
P3HT/CsGeI <sub>3</sub>	$1.0 \times 10^{12}$	0.6 eV	Neutral	$1.0 \times 10^{-19}$				
CsGeI <sub>3</sub> /TiO <sub>2</sub>	$1.0 \times 10^{12}$	0.6 eV	Neutral	$1.0 \times 10^{-19}$				
TiO <sub>2</sub> /FTO	$1.0 \times 10^{12}$	0.6 eV	Neutral	$1.0 \times 10^{-18}$				
CIGS/CdS	$1.0 \times 10^{10}$	0.6 eV	Neutral	$1.0 \times 10^{-19}$				
CdS/ZnO	$1.0 \times 10^{10}$	0.6 eV	Neutral	$1.0 \times 10^{-19}$				
ZnO/ZnO:Al	$1.0 \times 10^{11}$	0.6 eV	Neutral	$1.0 \times 10^{-18}$				

Figure 3. Calibration of (a) CsGeI<sub>3</sub> and (b) CIGS solar cells with experimental data to validate the simulated results.

distributions are  $\rho_p$  and  $\rho_n$ . The recombination rate is  $R$ , and hole and electron current densities are  $J_p$  and  $J_n$ . Electron and hole diffusion constants are  $D_n$  and  $D_p$ . Carrier generation rate is  $G$ , electron and hole mobilities are  $\mu_n$  and  $\mu_p$ , and electron and hole lifetimes are  $\tau_{n,p}$ . Thermal voltage is  $k_B T/e$ , light-generated current is  $I_L$ , saturation current is  $I_0$ , capture cross-section is  $\sigma$ , and total defect density is  $N_t$ . The tandem solar cell PCE is calculated from  $J_{SC}$ ,  $V_{OC}$ , FF, and incident power  $P_{in}$  from the equations (eqs 9 and 10).

$$PCE(\eta) = \frac{V_{oc} \times J_{sc} \times FF}{P_{in}} \quad (9)$$

$$FF = \frac{V_{max} \times J_{max}}{V_{oc} \times J_{sc}} \quad (10)$$

In Figure 2 the top and bottom solar cells (in the left side) are illuminated by direct incident and filtered AM 1.5G light spectrum (in the right side). The configuration is optimized to achieve its highest performance. The modified top cell includes a wide-bandgap lead-free perovskite CsGeI<sub>3</sub> absorber layer with a bandgap of 1.6 eV, flanked by P3HT as the hole transport layer (HTL) and TiO<sub>2</sub> as the electron transport layer (ETL).<sup>35,38,39</sup> Fluorine-doped tin oxide (FTO) serves as the transparent conducting layer for the front contact. The bottom CIGS cell has a 1.1 eV bandgap, absorbing light in the near- and far-infrared regions.<sup>44,59</sup> Aluminum and nickel are utilized for the front and back contacts for top and bottom solar cells, respectively. The

material parameters employed for simulating the top and bottom cells are summarized in Table 1. The simulation accounts for interface defect densities at both the HTL/perovskite and ETL/perovskite interfaces with a total defect density of approximately  $10^{12}$  cm<sup>-2</sup>. Additionally, defects are positioned at 0.6 eV above the valence band maximum (VBM) in the energy band structure. The top cell is exposed to the AM 1.5G solar spectrum, while the bottom CIGS cell receives the filtered spectrum transmitted from the top cell calculated with help of the following equations (eqs 11 and 12).<sup>60</sup>

$$S_{Ft}(\lambda) = S_{in}(\lambda) \times \exp\left\{-\sum_{k=1}^4 (\alpha_{mat_k}(\lambda) \times d_{mat_k})\right\} \quad (11)$$

where absorption coefficient ( $\alpha$ ) is given by

$$\alpha_{mat_k}(\lambda) = \left(\alpha_0 + \beta_0 \frac{E_G}{h\nu}\right) \sqrt{\left(\frac{h\nu}{E_g} - 1\right)} \quad (12)$$

In eq 11  $S_{Ft}(\lambda)$  is the transmitted filtered spectrum, and  $S_{in}(\lambda)$  is the AM 1.5 direct incident spectrum;  $\alpha$  represents absorption coefficient of material, and  $d_{mat}$  indicates the thickness of the specific material ( $mat_k = 1, 2, 3,$  and  $4$  for FTO, TiO<sub>2</sub>, CsGeI<sub>3</sub>, and P3HT, respectively). The absorption coefficient of each layer of the top cell is taken from the SCAPS database. The SCAPS database calculates the absorption coefficient with the help of eq 12, where  $\alpha_0 = 10^3/m$ ,  $\beta_0 =$

$10^{10}/\text{m}$ ,  $E_g$  is the bandgap of the material,  $h$  is Planck's constant, and  $\nu$  is the frequency of incident light.

**2.1. Calibration of Simulated Data with Experimental Works for Validation.** Before an in-depth analysis of the proposed tandem solar cell (TSC), the simulated results were validated through reported experimental data for CsGeI<sub>3</sub>-based PSCs and CIGS-based single-junction SCs. The top CsGeI<sub>3</sub> cell was initially calibrated to match experimental values, which reported a relatively low power conversion efficiency (PCE) of 4.94%, with  $J_{\text{SC}}$  of 18.11 mA/cm<sup>2</sup>,  $V_{\text{OC}}$  of 0.51 V, and a fill factor (FF) of 53.1% as depicted in Figure 3a.<sup>61</sup> The calibrated results are also shown in Table 2. Upon achieving

**Table 2. Calibration of the Cells and Comparison of Simulated Data with Experimental Findings**

Parameters	Experimental measurement (Under Direct illumination of AM1.5 G spectrum)	Calibrated Cell (Under Direct illumination of AM1.5 G spectrum)	Optimized Simulation (Top and bottom cell illuminated by Direct and Filtered AM 1.5 spectrum, respectively)
Top CsGeI <sub>3</sub> solar cell			
$V_{\text{OC}}$	0.51	0.52	1.06
$J_{\text{SC}}$	18.11	18.54	19.32
FF	53.1	52.06	82.04
$\eta$	4.94	4.96	16.93
Bottom CIGS solar cell			
$V_{\text{OC}}$	0.74	0.73	0.61
$J_{\text{SC}}$	38.50	39.98	19.31
FF	79.70	78.78	76.72
$\eta$	22.92	23.10	16.49

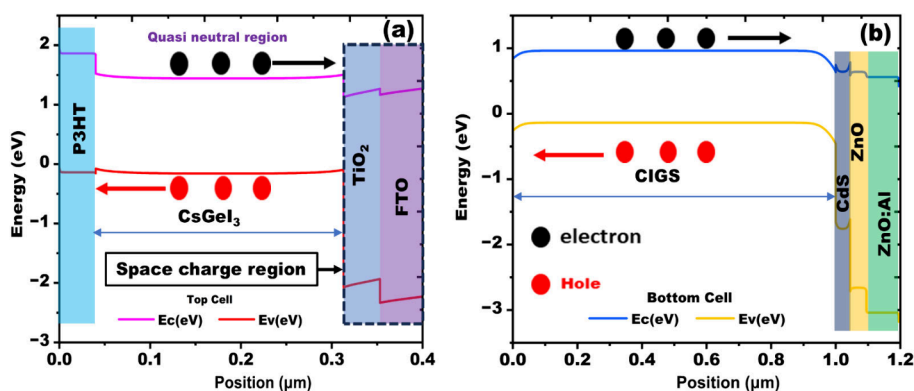
consistency with experimental results, the cell structure was modified by introducing a P3HT hole transport layer (HTL) to enhance the device performance. This approach to simulation calibration is consistent with prior studies.<sup>35,43</sup> The P3HT is selected due to its lower cost and superior ambient stability compared to Spiro-OMeTAD, which typically requires unstable dopants such as Li-TFSI and tBP that negatively affect device longevity. Moreover, P3HT exhibits favorable energy-level alignment with CsGeI<sub>3</sub>, promoting efficient hole extraction and reducing recombination losses.<sup>62,63</sup> In contrast, the bottom CIGS cell, calibrated with a thickness of 1000  $\mu\text{m}$  under direct AM 1.5 G spectrum, exhibited a PCE of 23.10% under AM 1.5 G illumination, closely aligning with the experimentally reported value of 22.92% as shown in Figure 3b.<sup>64</sup> After successful calibration of standalone solar cells, a filtered spectrum representative of light transmitted through the top cell was applied to the bottom cell, and simulation results were extracted. This methodology of calibrating simulations based on experimental data is well-supported in the literature.<sup>65–67</sup>

Calibration aligns simulation parameters with real-world conditions, minimizing performance prediction errors. Comparing simulated data to experimental results validates model accuracy, refines assumptions, and improves reliability. This iterative process enhances simulation credibility, enabling advancements in research and technology. Comparative analysis of calibrated parameters with experimental findings is presented in Table 2, while the J-V characteristics of both simulated and experimental CsGeI<sub>3</sub> and CIGS cells, shown in Figure 3a,b, confirm a strong correlation between simulated predictions and experimental data.<sup>43</sup>

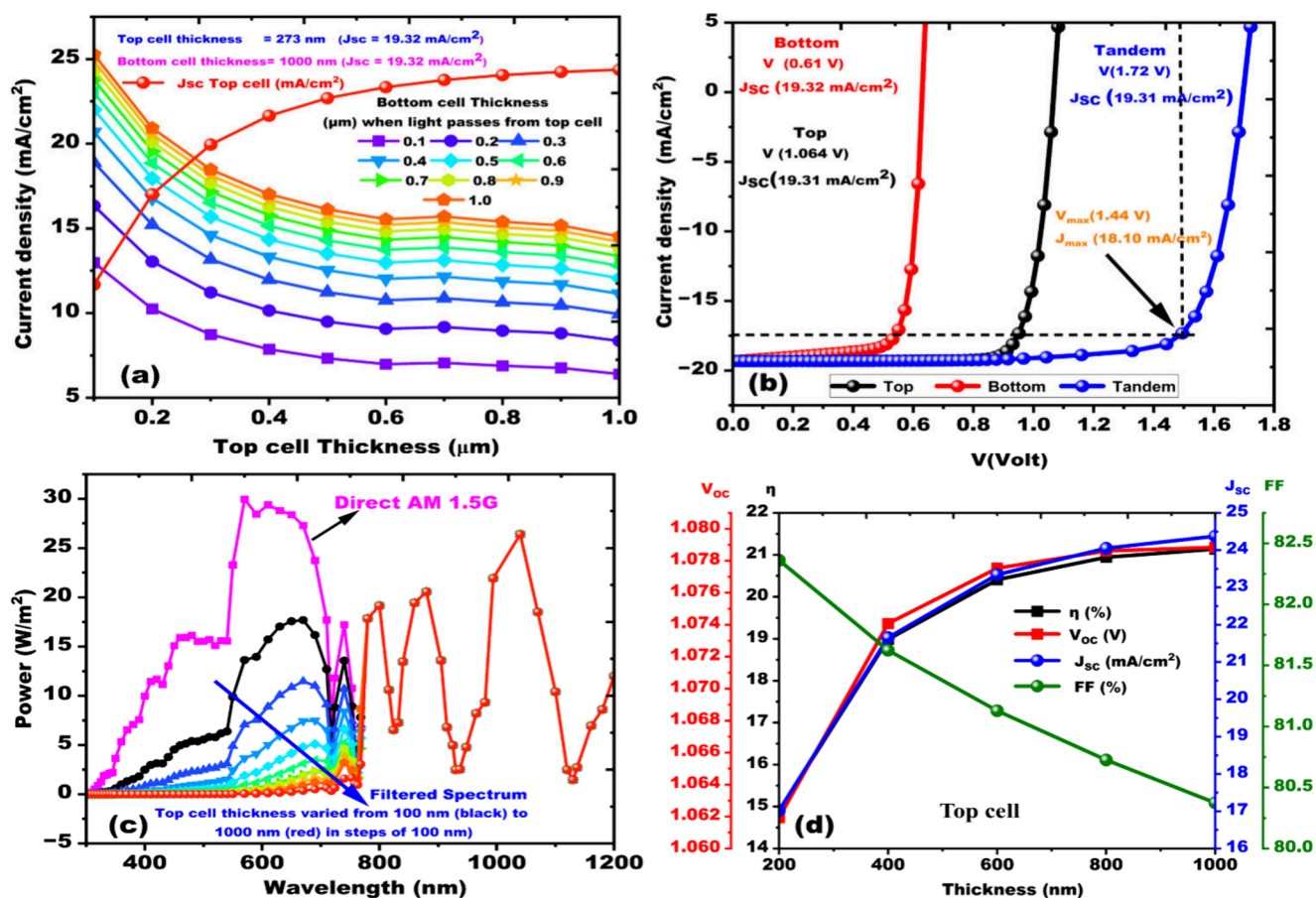
### 3. BAND DIAGRAM ANALYSIS OF THE TOP AND BOTTOM SOLAR CELL

Energy band diagrams (EBDs) of top and bottom subcells are very helpful to understand the charge carrier dynamics and band alignment of the PV performance of the device.<sup>68</sup> Space charge region or depletion region refers to a nonzero charge density region while a quasi neutral region has zero charge density region. Energy band alignment of the different layers utilized in the simulation is illustrated in Figure 4a,b, and this represents the electron affinity, energy of the valence band maxima, conduction band minima, and work function of the electrodes. When light shines on the solar cells, electron–hole pairs are generated and indicated by black and red colors, respectively, in Figure 4a,b. To separate these charge carriers for current flow, asymmetry in the semiconductor device is required, and P–N junction has such asymmetry which provides a built-in electric field at the junction.<sup>69</sup>

Under AM1.5G illumination at 300 K of the top solar cells, electron–hole pairs are generated in the SC's absorber layer and pass through the ETL and HTL to be collected at the contacts. The small conduction band offset ( $-0.38$  eV) at the TiO<sub>2</sub>/CsGeI<sub>3</sub> interface facilitates electron flow from the absorber to the FTO via TiO<sub>2</sub>. Conversely, the large valence band offset at the same interface hinders the hole flow to FTO. The higher conduction band offset between P3HT and CsGeI<sub>3</sub> blocks electron flow from the absorber to the contact. However, the P3HT's higher valence band energy level enables efficient hole extraction and transport. Furthermore, the ETL/absorber and absorber/HTL interfaces establish a strong electric field that promotes charge carrier separation and collection while impeding the flow of carriers with opposite charges.<sup>70</sup> In the bottom CIGS cell, filtered AM 1.5G light creates electron–hole pairs. The electric field at the CdS/CIGS interface separates these pairs, driving electrons to the ZnO:Al layer and holes to the CIGS layer for collection at the respective contacts.<sup>71</sup>



**Figure 4.** Standalone energy band diagrams of (a) P3HT/CsGeI<sub>3</sub>/TiO<sub>2</sub>/FTO and (b) CIGS/CdS/ZnO/ZnO:Al.



**Figure 5.** (a) Thickness variation of bottom solar cell from 0.1 to 1  $\mu\text{m}$  under filter spectrum to match  $J_{\text{SC}}$  of the top solar cell. (b) JV curve analysis of top, bottom, and TSC. (c) Filtered spectrum by changing the thickness of top solar cell absorber material shown by black to red graph and direct spectrum shown by pink color. (d) Impact of top cell absorber thickness on PV parameters.

## 4. RESULTS AND DISCUSSION

**4.1. JV Curve Analysis and Impact of Thickness on PV Parameters.** JV (current density–voltage) curves are essential for evaluating tandem solar cell performance, which arises from their stacked subcells' ability to absorb a broader solar spectrum. Analyzing the J-V curve allows researchers to optimize subcell materials, thicknesses, and bandgaps for improved current matching and higher efficiency. Figure 5a shows the current matching of both the top and bottom solar cell for making the 2T tandem device of CIGS and perovskite solar cells. As the thickness of the top and bottom cell increases from 0.1 to 1.0  $\mu\text{m}$ , then the  $J_{\text{SC}}$  starts to increase due to enhanced photon absorption and charge carrier generation. However, excessive thickness leads to increased recombination losses and series resistance, ultimately limiting the device performance. Mismatched currents cause energy losses and lower efficiency. The top and bottom cell absorber material thickness changes from 0.1 to 1.0  $\mu\text{m}$  under direct and filtered AM 1.5G spectrum as shown in Figure 5c, respectively. The maximum current matching condition is obtained at the optimized top and bottom solar cell thicknesses of 273 and 1000 nm, respectively. Current matching ensures equal contribution from both subcells, maximizing power production by balancing band gaps, thicknesses, and materials. Once the current matching condition is obtained, we make the two terminal tandem devices. Mismatched currents lead to energy losses, as the overall current is constrained by the weaker

subcells. Therefore, matching currents is crucial for a high-efficiency TSC. In 2T tandem configuration the maximum power is given by eq 13.<sup>55</sup>

$$P_{\text{max}} = (J_{\text{MPP}} \times V_{\text{MPP}}) \quad (13)$$

$J_{\text{MPP}}$  and  $V_{\text{MPP}}$  represent the current density and voltage at the maximum power point (MPP) of the TSC. The calculated values of the PV parameters from equations (eqs 9 and 10) of Top, Bottom, and TSCs are tabulated in Table 2. Figure 5b shows the individual J-V characteristics of top, bottom, and tandem solar cell with  $V_{\text{OC}}$  of 1.06, 0.61, and 1.73 V respectively. The J-V curves of the top subcells (measured under AM1.5G) and the bottom subcells (measured under a filtered spectrum) were distinctly obtained and combined in series at equal current. This approach ensures that the voltages are summed while maintaining current continuity, yielding the tandem J-V characteristics. The resulting tandem design demonstrates a remarkable conversion efficiency of 26.06%, a  $V_{\text{OC}}$  of 1.73 V, a  $J_{\text{SC}}$  of 19.32 mA/cm<sup>2</sup>, and a FF of 77.98%, highlighting its potential for high-performance photovoltaic applications.

Table 3 shows that the top and bottom solar cells have photoconversion efficiencies of 16.93% and 16.49%, respectively. The higher  $J_{\text{SC}}$  observed in Table 3 likely results from the tandem structure's improved optical and electrical design. This includes enhanced light absorption from optimized layer thicknesses, reduced recombination losses at interfaces, and efficient charge extraction. Improved band alignment between

Table 3. PV Parameters of Top, Bottom, and TSCs

PV Parameters	$V_{OC}$ (V)	$J_{SC}$ (mA/cm <sup>2</sup> )	FF (%)	PCE (%)
Top	1.06	19.31	82.04	16.93
Bottom	0.61	19.32	76.72	16.49
Tandem	1.73	19.32	77.98	26.06

subcells may also facilitate better carrier transport, contributing to the higher  $J_{SC}$ . The similarity in these efficiencies results from optimizing the bandgap of top and bottom solar cells, current matching, and minimizing optical and electrical losses, consistent with previously published work.<sup>72,73</sup>

Figure 5d shows the impact of top cell absorber material thickness on the standalone top PSC's PV parameters as the CsGeI<sub>3</sub> layer thickness varies from 200 to 1000 nm. As the absorber layer thickness increases, the short-circuit current density ( $J_{SC}$ ) of the cell increases significantly before saturating. In contrast, the open-circuit voltage ( $V_{OC}$ ) shows a slight increase from 1.060 to 1.078 V within the 100 nm–800 nm thickness range, also saturating with further increases in CsGeI<sub>3</sub> layer thickness. The thicker absorber layer enhances the photon absorption, boosting the photocurrent. However, increased thickness also leads to greater bulk recombination, which limits  $V_{OC}$ .<sup>74</sup> Figure 5d illustrates that the fill factor (FF) declines linearly with increasing CsGeI<sub>3</sub> layer thickness due to rising series resistance ( $R_s$ ), while the power conversion efficiency (PCE) trends similarly to  $J_{SC}$ , peaking at approximately 20.8% for absorber layer thicknesses between 800 and 1000 nm.

**4.2. QE Characteristic of Optimized Top and Bottom Solar Cell.** Quantum efficiency is defined as the ratio of total number of electron hole pair generation to total number of photons incident into the solar cell. However, the conversion of photons into electrons at a given wavelength differs from the number of electrons successfully collected in the device electrode due to recombination losses and unabsorbed photon loss. External quantum efficiency (EQE) considers all incident light, while internal quantum efficiency (IQE) considers only absorbed photons. QE is crucial for assessing a solar cell's spectral response and overall performance.<sup>75</sup> QE is measured in short-circuit mode by determining the short-circuit current for monochromatic incident light. SCAPS measures the EQE because it considers the full device response to incident photons, including recombination losses but not optical reflection losses.<sup>60</sup>

The EQE of the solar cell is given by eq 14.

$$EQE = \frac{\Delta J_{SC}}{q \Delta \Phi_{\lambda}} \quad (14)$$

Here,  $\Delta J_{SC}$  denotes the change in short-circuit current induced in a solar cell by a change in photon flux  $\Delta \Phi_{\lambda}$  at wavelength  $\lambda$ . Figure 6a,b shows wavelength ranges of 300–800 nm for the top PSC and 300–1200 nm for the bottom CIGS cells. It is observed that increased thickness in both cells led to higher quantum efficiency (QE). The reason is that a thicker layer enhances light absorption, especially for longer wavelengths that penetrate more deeply. This reduces the chance of photons passing through without being absorbed, thereby minimizing transmission losses. Increased photon absorption generates more electron–hole pairs, enhancing the charge carrier generation. Furthermore, a thicker absorber better utilizes the broader solar spectrum, capturing a wider range of wavelengths.<sup>76,77</sup> The QE of the top cell at a thickness of 1  $\mu\text{m}$  varies from 97.76% to 56.88% in the wavelength range of 300–770 nm and drops to zero thereafter under the condition of negligible series resistance and very high shunt resistance. Similarly at bottom cell thickness of 2.1  $\mu\text{m}$  the optimum values of QE were obtained in the range of 520 to 1100 nm under the similar condition of resistances, as shown in Figure 6 b.

**4.3. Influence of the Series Resistance ( $R_s$ ) and Shunt Resistance ( $R_{sh}$ ) on PV Parameters and JV Characteristics.** This section examines the effects of  $R_s$  and  $R_{sh}$  on solar cell performance. Series resistance encompasses resistances from semiconductor and metal contact points along the current path, and shunt resistance is caused by leakage current across the  $P$ – $N$  junction due to shunts at the cell periphery, crystal defects, or impurity precipitates. The two-diode model equivalent circuit of the solar cell including parasitic resistance is shown in Figure 9.  $R_s$  varies from 0.5  $\Omega\cdot\text{cm}^2$  to 5  $\Omega\cdot\text{cm}^2$ , while  $R_{sh}$  ranges from 10  $\Omega\cdot\text{cm}^2$  to 10<sup>8</sup>  $\Omega\cdot\text{cm}^2$ , allowing one to analyze the simultaneous effects of both parameters on PV performance through contour mapping, as shown in Figure 7a,b,c,d.

From Figure 7a it is observed that  $V_{OC}$  changes from 0.19 to 1.07 V, in Figure 7b  $J_{SC}$  changes from 12.86 mA/cm<sup>2</sup> to 19.32 mA/cm<sup>2</sup>, in Figure 7c FF changes from 25% to 82.20%, and in Figure 7d PCE changes from 0.6% to 16.95% as  $R_s$  and  $R_{sh}$  simultaneously change from 0.5  $\Omega\cdot\text{cm}^2$  to 5  $\Omega\cdot\text{cm}^2$  and from 10 to 10<sup>8</sup>  $\Omega\cdot\text{cm}^2$ , respectively. Very large  $R_s$  and very low  $R_{sh}$  represent the straight line in the J-V curve of Figure 8a,b. Hence from Figures 7 and 8 it is concluded that a low value of

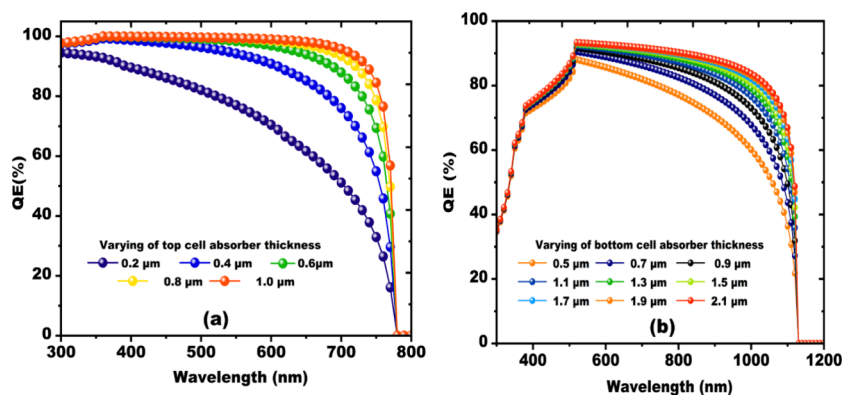


Figure 6. QE analysis by varying thickness of (a) top cell absorber and (b) bottom cell absorber

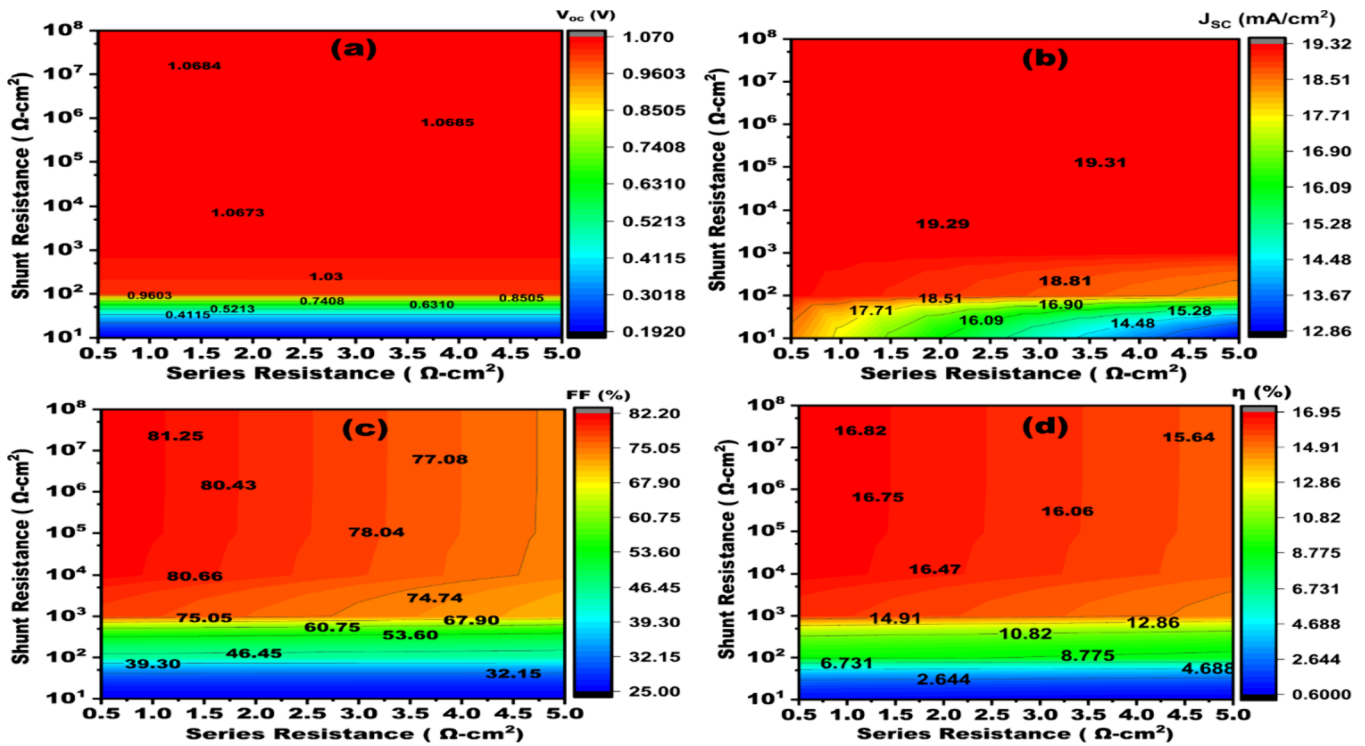


Figure 7. Parasitic resistance impact on the top cell of the PV parameters (a)  $V_{OC}$ , (b)  $J_{SC}$ , (c) FF, (d)  $\eta$ .

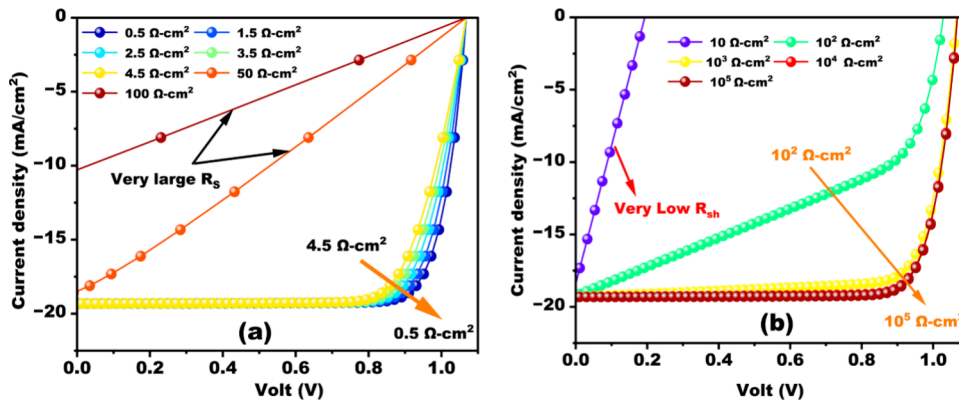


Figure 8. Effect of (a) series resistance and (b) shunt resistance on the fill factor (observe the squareness of J-V Curve) of the top solar cell.

$R_S$  ( $<0.5 \Omega\text{-cm}^2$ ) and high value of  $R_{Sh}$  ( $>10^3 \Omega\text{-cm}^2$ ) are desirable.<sup>78,79</sup> Figure 8a,b illustrates how  $R_S$  and  $R_{Sh}$  affect the squareness of the J-V curve in relation to the fill factor.

The squareness of the JV curve affects the fill factors, and it is given in terms of the parasitic resistance through equations (eqs 15 and 16).<sup>80–82</sup>

$$FF = FF_0(1 - r_s) \quad (15)$$

$$FF = FF_0 \left( 1 - \frac{1}{r_{sh}} \right) \quad (16)$$

Where  $FF_0$  represents ideal fill factor in the absence of any parasitic resistance,  $r_s = R_S/R_{ch}$  and  $r_{sh} = R_{sh}/R_{ch}$  are normalized series and shunt resistance, respectively, and the term  $R_{ch}$  ( $R_{ch} = V_{OC}/I_{SC}$ ) represents the characteristic resistance of the solar cells.

The two-diode model of the solar cell circuit diagram accurately represents electrical behavior by accounting for

nonideal effects such as recombination losses and leakage currents. This model is crucial for optimizing solar cell design and enhancing efficiency, offering a thorough understanding of the performance under real-world conditions. In Figure 9,  $J_{01}$  and  $J_{02}$  represent the saturation current densities as a recombination in base emitter and space charge region,  $I$  is the current across  $R_S$ , and  $V$  is the output voltage.

**4.4. Impact of Temperature and Absorption Coefficients of Top Cell.** Figure 10a depicts the J-V curve performance of tandem solar cell for different temperatures. Solar cell performance declines with rising temperature primarily due to increased internal carrier recombination driven by higher carrier concentrations. This reduces the built-in potential across the  $P-N$  junction, which lowers the open-circuit voltage ( $V_{OC}$ ). Operating temperature is therefore critical for photovoltaic conversion.<sup>83–87</sup> The temperature dependence of the solar cell performance comes from the dependency of  $V_{OC}$  on temperature that depends on the reverse saturation current ( $I_0$ ) according to eq 17.

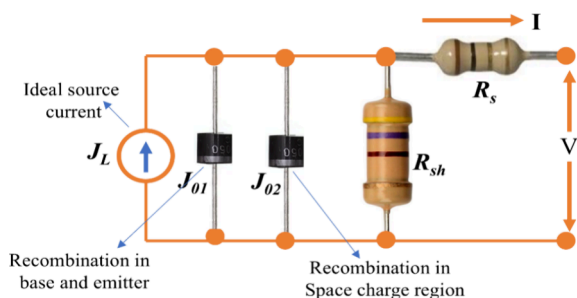


Figure 9. Two-diode model equivalent circuit of the solar cell.

$$I_0 \propto e^{-E_g/kT} \quad (17)$$

In Figure 10a, device performance is analyzed by varying the operating temperature from 300 to 400 K. The plot indicates that  $V_{OC}$  decreases as temperature increases, likely due to the rise in intrinsic carrier concentration ( $n_i$ ) and resulting increase in reverse saturation current. Intrinsic carrier density is dependent on the semiconductor material's bandgap energy ( $E_g$ ) and temperature ( $T$ ) given by eq 18, and the expression for  $V_{OC}$  is given by eq 19.<sup>88</sup>

$$n_i^2 \propto e^{-E_g/kT} \quad (18)$$

$$V_{OC} = \frac{kT}{q} \times \ln \frac{I_{SC}/I_0}{q} \quad (19)$$

In Figure 10a the area under the JV curve decreases as temperature increases, which reduces the open-circuit voltage and hence the overall performance of the SC affected. Figure 10b indicates that the absorption coefficients of each layer of the top solar cell were calculated from eq 12 and later these coefficients are used for calculation of the filtered spectrum to study the bottom cell performance. The absorption coefficient quantifies how deeply light of a given wavelength penetrates a material before being absorbed. Different wavelengths penetrate at different depths, impacting the generation of electron–hole pairs. The graph demonstrates that even above the band gap, the absorption coefficient varies significantly with wavelength. Photon absorption depends on the probability of a photon interacting with an electron to facilitate a transition between energy bands. Near the band gap energy, absorption is lower because only electrons at the valence band edge can participate. As photon energy increases beyond this,

more electrons become capable of interaction, leading to higher absorption.<sup>89,90</sup>

## 5. COMPARISON TO SIMILAR WORKS

This work focuses on the optimization of an environmentally friendly CsGeI<sub>3</sub>/CIGS tandem solar cell, aiming to establish it as a potential alternative to its lead-based counterparts. The performance potential is evaluated using four key parameters:  $J_{SC}$ ,  $V_{OC}$ , FF, and PCE, benchmarked against recently reported values in the literature. For comparison, in the earliest published work the highest reported  $J_{SC}$ ,  $V_{OC}$ , FF, and PCE for a Pb-based perovskite/CIGS tandem solar cell are 19.24 mA/cm<sup>2</sup>, 1.768 V, 72.9%, and 24.2%.<sup>91</sup> In this work, the CsGeI<sub>3</sub>/CIGS tandem achieved  $J_{SC}$ ,  $V_{OC}$ , FF, and PCE values of 19.32 mA/cm<sup>2</sup>, 1.73 V, 77.98%, and 26.06%, respectively. Additionally, when compared to the Shockley–Queisser (SQ) limit (~33%) for a single-junction solar cell with a 1.1 eV bandgap (CIGS), the proposed tandem device shows nearly 0.41%, 6.51%, and 7.13% improvement in  $J_{SC}$ , FF, and PCE, respectively, while  $V_{OC}$  reduces to 2.14%. The one possible reason could be for decrease in  $V_{OC}$  is higher nonradiative recombination particularly at interfaces and defects, lowering  $V_{OC}$  by reducing charge carrier lifetime. High series resistance in contacts or layers can limit charge extraction, negatively impacting  $V_{OC}$ . A comprehensive comparison of this work to similar reports in the literature is shown in Table 4.

Table 4. Comparison of Current Work with Earlier Published Work

Top/Bottom subcells	$V_{OC}$ (V)	$J_{SC}$ (mA/cm <sup>2</sup> )	FF (%)	PCE (%)	ref
CIGS/CsGeI <sub>3</sub>	1.73	19.32	77.98	26.06	This work
Cs(MAFA)Pb(IBr)/CIGS	1.04	19.24	72.9	24.2	91
CIGS/Cu <sub>2</sub> ZnSn(S,Se) <sub>4</sub>	1.45	16.1	68.2	15.90	92
CsGeI <sub>3</sub> /c-Si	1.90	17.55	84.9	28.43	35
CIGS/SWCNT	1.34	37.87	76.41	38.91	66
CIGS/Si	1.45	16.70	81.50	19.80	93
CsGeI <sub>3</sub> /FASnI <sub>3</sub>	2.12	16.71	85.87	30.42	38
CsGeI <sub>3</sub> /CsGeI <sub>2</sub> Br	1.22	32.79	79.19	31.86	42
CsGeI <sub>3</sub> /CsPbI <sub>3</sub>	1.04	20.70	67.72	14.63	94

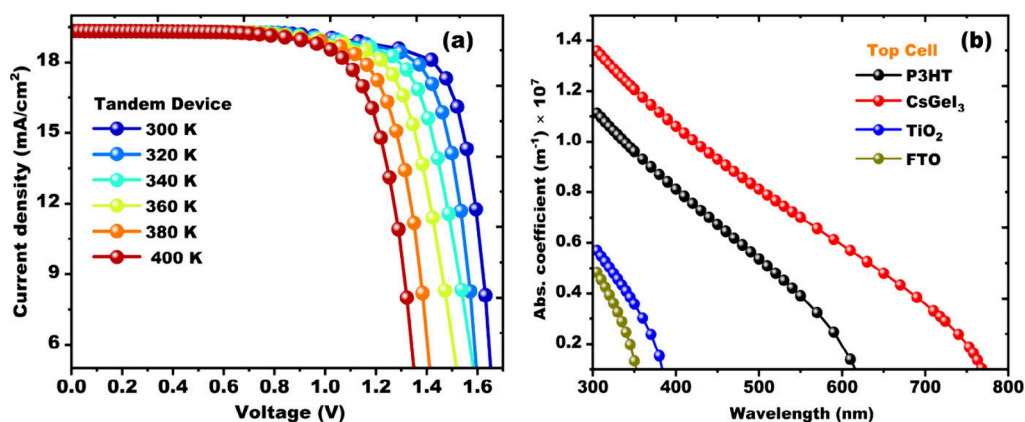


Figure 10. (a) Impact of temperature on J-V characteristics of tandem solar cell. (b) The absorption coefficient analysis for top solar cell layers including P3HT, CsGeI<sub>3</sub>, TiO<sub>2</sub>, and FTO used during simulation and for calculation of filtered spectrum (Taken from SCAPS database file).

The performance parameters of the CIGS/CsGeI<sub>3</sub> solar cell reported in this work showcase a significant position among the tandem solar cells reported in the literature.

## 6. CONCLUSIONS

This work concludes the photovoltaic performance of a two-terminal CsGeI<sub>3</sub>/CIGS tandem solar cell (TSC) that demonstrates a power conversion efficiency (PCE) of 26.06% ( $J_{SC} = 19.32 \text{ mA/cm}^2$ ,  $V_{OC} = 1.73 \text{ V}$ ,  $FF = 77.98\%$ ), establishing it as a promising lead-free alternative for high-efficiency photovoltaics. Optimized standalone top and bottom cell thicknesses of 273 and 1000 nm absorber layers achieved PCEs of 16.93% and 16.49%, respectively. The simulations were calibrated with experimental data for both cells to ensure the accuracy of the simulation and were also compared with the experimental findings. This study investigates the impact of various parameters, including layer thickness, parasitic resistance, temperature, quantum efficiency, band diagram, absorption coefficients, and two-diode model equivalent circuit, on the solar cell performance. This tandem design presents a pathway for developing efficient and cost-effective perovskite-CIGS tandem solar cells, with the reported performance representing a record for this device structure and a potential alternative to lead-free tandem solar cells. Future work may explore the impact of the tunnel recombination junction. We also believe that our approach will advance high-performance PSC/CIGS tandem solar cell development and broaden their application in building-integrated photovoltaics.

## ■ ASSOCIATED CONTENT

### Data Availability Statement

Data will be made available on request.

## ■ AUTHOR INFORMATION

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### Notes

The authors declare no competing financial interest.

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