

Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells

Ritu Paliwal¹, , Subhash C. Yadav², Yugal S. Kasana¹, Jagdish P. Yadav¹, Nidhi Agrawal¹, Dinesh K. Yadav¹, Balram Tripathi³, Jitendra K. Mishra¹

1. Department of Physics, University of Rajasthan, Jaipur, IND

2. Department of Advanced Science and Technology, Toyota Technological Institute, Nagoya, JPN

3. Department of Physics, S.S. Jain Subodh P.G. College, Jaipur, IND

Received: April 16, 2026 | Review began: April 17, 2026 | Review ended: May 17, 2026 | Published: June 17, 2026

© Copyright 2026

This is an open access article distributed under the terms of the Creative Commons Attribution License CC-BY 4.0., which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

Abstract

The performance limitations of single-absorber perovskite solar cells caused by spectral losses can be reduced by adopting dual-absorber architectures capable of harvesting a broader solar spectrum. In this study, a lead-free dual-absorber device employing $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ and Sr_3SbI_3 as complementary absorber layers is theoretically investigated using Solar Cell Capacitance Simulator in 1D simulation tool. The effects of absorber thickness, defect density, and doping concentration on photovoltaic performance are systematically analyzed.

The optimized dual-absorber device achieved a maximum theoretical power conversion efficiency (PCE) of 35.22%, which is higher than the 30.11% obtained for the single-absorber $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ device under near-ideal defect conditions. Under realistic defect densities, the simulated device exhibited a PCE of 21.19%. The results identify absorber defect density as the dominant factor governing device performance due to trap-assisted recombination. A temperature-dependent analysis was also performed to evaluate realistic operating conditions. These findings provide simulation-guided insights for the design of stable and efficient lead-free dual-absorber perovskite solar cells.

Categories: Advanced Materials, Materials Engineering, Energy Efficiency and Conservation

Keywords: dual-absorber architectures, perovskite solar cells, scaps-1d, cesium copper antimony chloride, strontium antimony iodide

Introduction

Within just a decade, perovskite solar cells (PSCs) have shown great potential, outperforming market-dominant silicon photovoltaics. The perovskite materials possess an ABX_3 type chemical structure, where A and B represent a univalent and a divalent cation, respectively, and x signifies a halide ion [1,2]. Besides having superior optoelectronic attributes, including a high panchromatic light absorption coefficient [3], an adjustable bandgap [2], low excitonic binding energy [4], and extended charge carrier diffusion lengths [5], these properties can also be tuned by substitution of their constituent ions, and thereby making them suitable for advanced applications [6]. Recent research findings have demonstrated a record power conversion efficiency (PCE) of over 26% for single-junction PSCs [7]. However, these high

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. Cureus J Eng 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

performing-materials contain lead (Pb) as the divalent cation, which is hazardous from an environmental aspect [8]. As an alternative approach, the Pb^{2+} ion can be replaced by Sn^{2+} or Ge^{2+} , but the oxidation tendency of these cations, owing to elevated energy levels of the 5s and 4s orbitals, influences the durability of PSCs [9]. Therefore, non-toxic low-dimensional (2D and 0D) perovskites were synthesized by using heterovalent Bi^{3+} and Sb^{3+} substitutes for Pb^{2+} . However, non-ideal optoelectronic properties, such as an indirect band gap and low carrier mobilities, limit their practical application in optoelectronic devices [10-13]. Subsequently, the double perovskite structure $\text{A}_2\text{BB}'\text{X}_6$, where A represents a monovalent cation, B denotes a monovalent metal ion, B' correspond to a trivalent metal ion, and X is a halide ion, has garnered significant attention as a promising candidate obtained by replacing Pb^{2+} with a monovalent and trivalent cation [14,15]. Despite exhibiting high structural stability and non-toxicity, the indirect wide band gap of these materials obstructs their widespread applicability in photovoltaics [16].

Concurrently, layered double perovskite-structured materials have emerged as novel contenders, where the intrusion of a divalent transition metal ion in the double perovskite structure disrupts the 3D network and leads to the formation of layered structure [17]. Vargas et al. synthesized earth abundant and non-toxic $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ (CCSC) layered double perovskite material, having a band gap of ~ 1 eV [18]. However, the bulk material possesses an indirect band gap and a higher electron effective mass. Later, Wang et al. reported fabrication of single-layer CCSC nanocrystals having a direct band gap (1.6 eV) and lower electron effective mass. Moreover, unlike Pb-halide perovskites, CCSC demonstrates stability in various polar solvents. While CCSC dissociates into $\text{Cs}_3\text{Sb}_2\text{Cl}_9$, Cs_2CuCl_4 and SbCl_3 at 210°C , the degradation is reversible under high humidity and low temperature conditions [17]. Still, the material exhibits superior optoelectronic properties, thermal and chemical stability compared to conventional hybrid lead halide perovskite materials. Recent studies emphasize the design and optimization of CCSCNCs based PSCs [19]. Despite notable performance gains, spectral losses still limit the efficiency of single junction devices, leaving considerable room for further advancement pathways. This limitation has enabled the exploration of double-absorber structures, facilitated a broader solar spectrum absorption and thereby mitigating energy losses. In this regard, Sr_3SbI_3 , having direct band gap of ~ 1.31 eV, can be chosen as bottom absorber owing to its favorable band gap, compositional, and heat stability [20]. Moreover, inorganic metal oxide layers are the most suitable as charge transport layers due to their stability, earth abundance, high performance, and manufacturing compatibility. However, prior to experimental fabrication, theoretical modeling of device operational parameters, such as PCE, short circuit current density (J_{sc}), open circuit voltage (V_{oc}), and fill factor (FF) via optimization of thickness, defect densities, and doping concentration is highly beneficial to evaluate device performance and feasibility. In this context, multiple software tools such as, SILVACO ATLAS [21], SETFOS [22], wxAMPS [23], and finite difference time domain method [24], and others are used for the simulation of solar cells, which generally rely on solving fundamental second-order differential equations of semiconductors employing appropriate interfacial boundary conditions. Among all these computational software packages, the Solar Cell Capacitance Simulator in 1D (SCAPS-1D) is widely utilized for heterojunction and multijunction simulations [25].

The present study employs SCAPS-1D software program to assess the $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ and Sr_3SbI_3 double absorber device performance utilizing cost-effective inorganic TiO_2 and Cu:NiO as Electron Transport Layer (ETL) and Hole Transport Layer (HTL), respectively, with the device architecture of $\text{FTO}/\text{TiO}_2/\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3/\text{Cu:NiO}/\text{Au}$. The aim is to evaluate the influence of dual-layer implementation in improving the device performance relative to the single-layer device structure under optimized layer parameters. The simulated device exhibited the maximum PCE of 35.22% under optimized values of thickness, doping, and defect concentrations. In addition, the effect of temperature is also studied, estimating the real-world operational performance of the designed device.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. *Cureus J Eng* 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

Materials And Methods

All simulations were performed under standard AM 1.5G illumination using SCAPS-1D, assuming ohmic contacts and bulk-limited recombination within the absorber layers. Figure 1 shows the n-i-p structured device architectures employing $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ and $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ as absorbers. The fluorine-doped tin oxide (FTO) coated glass is adopted as a transparent conducting substrate owing to its chemical inertness and high thermal stability. The TiO_2 layer is implemented as an electron transport (and hole-blocking) layer due to its favorable energy level alignment, high conductivity, high carrier mobility, and low-temperature processing [26]. Cu-doped NiO (Cu:NiO) is used as the HTL owing to its stability, high conductivity, and abundance [27].

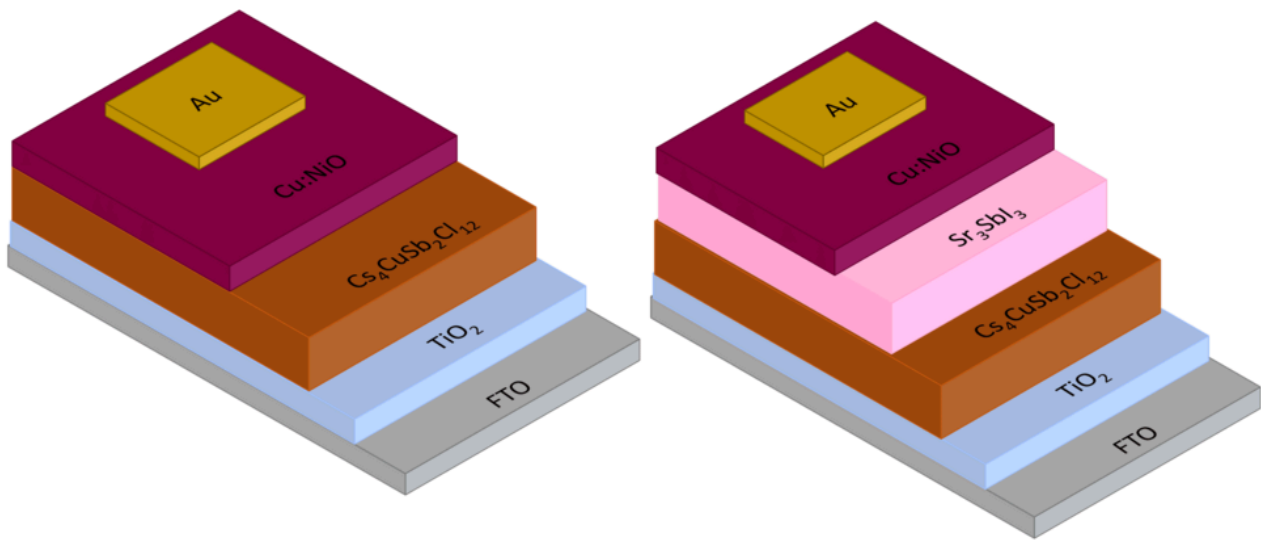


FIGURE 1: Diagrammatic illustration of n-i-p structured perovskite solar cell device framework

FTO, fluorine-doped tin oxide

In addition, gold (Au) is utilized as back electrode throughout the procedure owing to its high electrical conductivity, suitable work function, and excellent chemical stability. The standard AM 1.5 solar spectrum at 1000 Wm^{-2} irradiation intensity is adopted for entire simulation. The charge carrier dynamics in semiconductors is determined by the three fundamental equations listed below [28].

$$\frac{dy}{dx} = -\frac{d^2\psi}{dx^2} = \frac{q}{\epsilon} [p(x) - n(x) + N_D^+(x) - N_A^-(x) - n_t(x) + p_t(x)] \quad (1)$$

$$\frac{dn_p}{dt} = G_n - \frac{n_p - n_{p0}}{\tau_n} + n_p \mu_n \frac{dE}{dx} + D_n \frac{d^2 n_p}{dx^2} + \mu_n E \frac{dn_p}{dx} \quad (2)$$

$$\frac{dp_p}{dt} = G_p - \frac{p_p - p_{p0}}{\tau_p} + p_p \mu_p \frac{dE}{dx} + D_p \frac{d^2 p_p}{dx^2} + \mu_p E \frac{dp_p}{dx} \quad (3)$$

Equation (1) is known as the Poisson equation, where Ψ , ϵ , and q correspond to the electrostatic potential, the permittivity of semiconductor material, and the electron charge, respectively. Further, n , p , N_D^+ , and N_A^- are the concentrations of electron, hole, ionized acceptor, and ionized donor, respectively, n_t and p_t are the trapped electron and

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. *Cureus J Eng* 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

hole concentrations, and x is position coordinate. The continuity equations governing the transport of electrons and holes are represented in equations (2) and (3). Here G_n and G_p indicate electron and hole generation rates, n_p and p_n correspond to electron and hole concentrations, n_{p0} and p_{n0} signify electron and hole concentrations at equilibrium in p and n-regions, τ_n and τ_p represent electron and hole lifetimes. D_n and D_p represent the diffusion coefficients of electrons and holes, μ_n and μ_p are electron and hole mobilities and E corresponds to the external electric field. Similarly, the following equations govern the charge dynamic mechanism through drift and diffusion.

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

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

Here E_{Fn} and E_{Fp} represent the electron and hole quasi-Fermi energy levels. Tables 1 and 2 tabulate the material parameters required to simulate PSCs.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of Cs₄CuSb₂Cl₁₂/Sr₃SbI₃ Dual Absorber Lead-Free Perovskite Solar Cells. Cureus J Eng 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

Material parameters	FTO	TiO ₂	Cs ₄ CuSb ₂ Cl ₁₂	Sr ₃ SbI ₃	Cu: NiO
Thickness (nm)	200	50 [*]	700 [*]	700 [*]	50
Band gap (eV)	3.5	3.2	1.6	1.31	3.55
Dielectric constant	9.0	9.0	10.0	5.4	11.75
Electron affinity (eV)	4.0	4.0	3.74	4.0	1.8
Effective density of states at CB (cm ⁻³)	2.2×10^{18}	1×10^{18}	4.5×10^{19}	1.2×10^{19}	2.2×10^{21}
Effective density of states at VB (cm ⁻³)	1.8×10^{19}	1.8×10^{19}	1.6×10^{19}	2.4×10^{19}	1.8×10^{19}
Electron mobility (cm ² /V-s)	20	20	2.5	50	1.5×10^{-2}
Hole mobility (cm ² /V-s)	10	10	2.5	25	1.5×10^{-2}
Thermal velocity (electrons) (cm/s)	10^7	10^7	10^7	10^7	10^7
Thermal velocity (holes) (cm/s)	10^7	10^7	10^7	10^7	10^7
Doner density (N _D) (cm ⁻³)	1×10^{15}	$1.8 \times 10^{19*}$	0	0	0
Acceptor density (N _A) (cm ⁻³)	0	0	10^{13}	10^{17}	10^{18}
Total defect density (cm ⁻³)	-	10^{15}	10^{13*}	10^{12*}	10^{16}
References	[25]	[29]	[30]	[31]	[32]

TABLE 1: Material parameter inputs used in present study

FTO, fluorine-doped tin oxide.

Here (*) indicates the variation in particular input parameter.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of Cs₄CuSb₂Cl₁₂/Sr₃SbI₃ Dual Absorber Lead-Free Perovskite Solar Cells. Cureus J Eng 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

Input parameters	TiO ₂	Cs ₄ CuSb ₂ Cl ₁₂	Sr ₃ SbI ₃	Cu: NiO
Defect types	Neutral	Neutral	Neutral	Neutral
Electrons/holes capture cross-section (cm ⁻²)	1.0 × 10 ⁻¹⁵	1.0 × 10 ⁻¹⁵	1.0 × 10 ⁻¹⁵	1.0 × 10 ⁻¹⁵
Energy distributions	Uniform	Uniform	Uniform	Uniform
Defect energy level reference (E _r)	Above VB maximum	Above VB maximum	Above VB maximum	Above VB maximum
Energy level relative to reference (eV)	0.6	0.6	0.6	0.6
Characteristic energy (eV)	0.1	0.1	0.1	0.1

TABLE 2: Input parameters utilized in device simulation

Results And Discussion

The high performance of PSCs necessitates the thickness optimization of constituent layers, including the perovskite absorbing layer, the n-type TiO₂ layer, and the p-type Cu: NiO film. Figure 2a shows the effect of Cs₄CuSb₂Cl₁₂ thickness modulation on device operational parameters. The increase in thickness leads to a slight increase in PCE, but after a certain thickness, it saturates due to increased bulk recombination losses. Along with absorber layer thickness, bulk defect density is also a dominant factor governing device performance, as demonstrated by Figure 2b. On varying the absorber bulk defect density from 10¹¹ cm⁻³ to 10¹⁵ cm⁻³, the PCE decreases as defect density increases, resulting from a decline in V_{oc} and fill factor due to enhanced trap assisted losses. At optimized defect concentration 10¹¹ cm⁻³, the simulated Cs₄CuSb₂Cl₁₂ based device attained a maximum PCE of 30.11%.

How to cite this article:

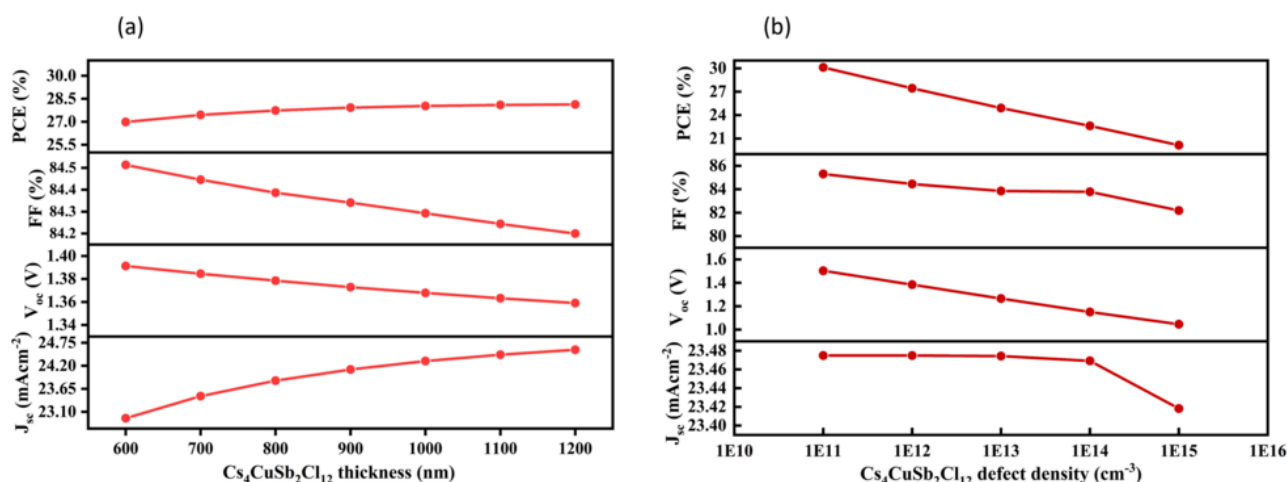


FIGURE 2: Device operational parameters variation with (a) thickness and (b) bulk defect density of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ absorbing layer

PCE, power conversion efficiency; FF, fill factor

This PCE can be increased further by implementing a dual layer architecture, employing Sr_3SbI_3 as narrow band gap absorber owing to increased solar absorption. Still, the optimum performance of this dual-layer device necessitates optimization of the subsequent layer parameters. Figure 3 shows the negligible variation in the solar cell parameters upon varying the thickness of the TiO_2 hole blocking layer from 30 nm to 100 nm. Although the wide-bandgap ETL also serves as a UV filter for the underlying perovskite layer, a thicker ETL may lead to increased parasitic irradiative losses and series resistance. Also, an excessively thin ETL causes pinholes and low reproducibility, thereby an optimum thickness is essential for better device performance.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. *Cureus J Eng 3* : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

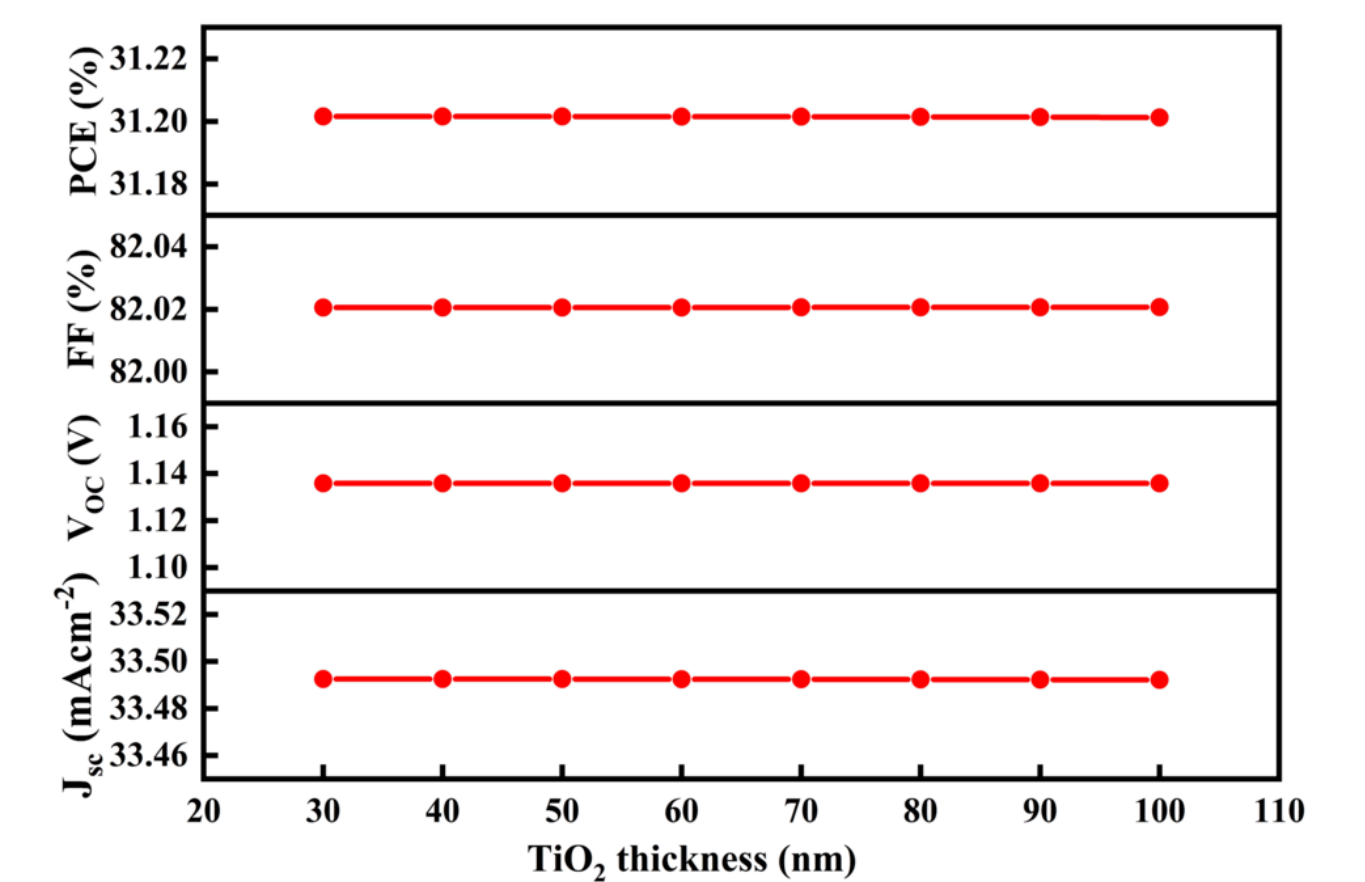


FIGURE 3: Device parameters with variation in TiO₂ layer thickness

PCE, power conversion efficiency; FF, fill factor

Similarly, Figure 4 illustrates the effect of relative thickness variation of Cs₄CuSb₂Cl₁₂ and Sr₃SbI₃ perovskite layers from 600 nm to 1200 nm on the device parameters. At a constant thickness of Sr₃SbI₃, PCE decreases on increasing the thickness of Cs₄CuSb₂Cl₁₂ layer. With increasing Sr₃SbI₃ thickness, the PCE initially increases, attains a maximum value, and subsequently decreases upon further thickness enhancement.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of Cs₄CuSb₂Cl₁₂/Sr₃SbI₃ Dual Absorber Lead-Free Perovskite Solar Cells. Cureus J Eng 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

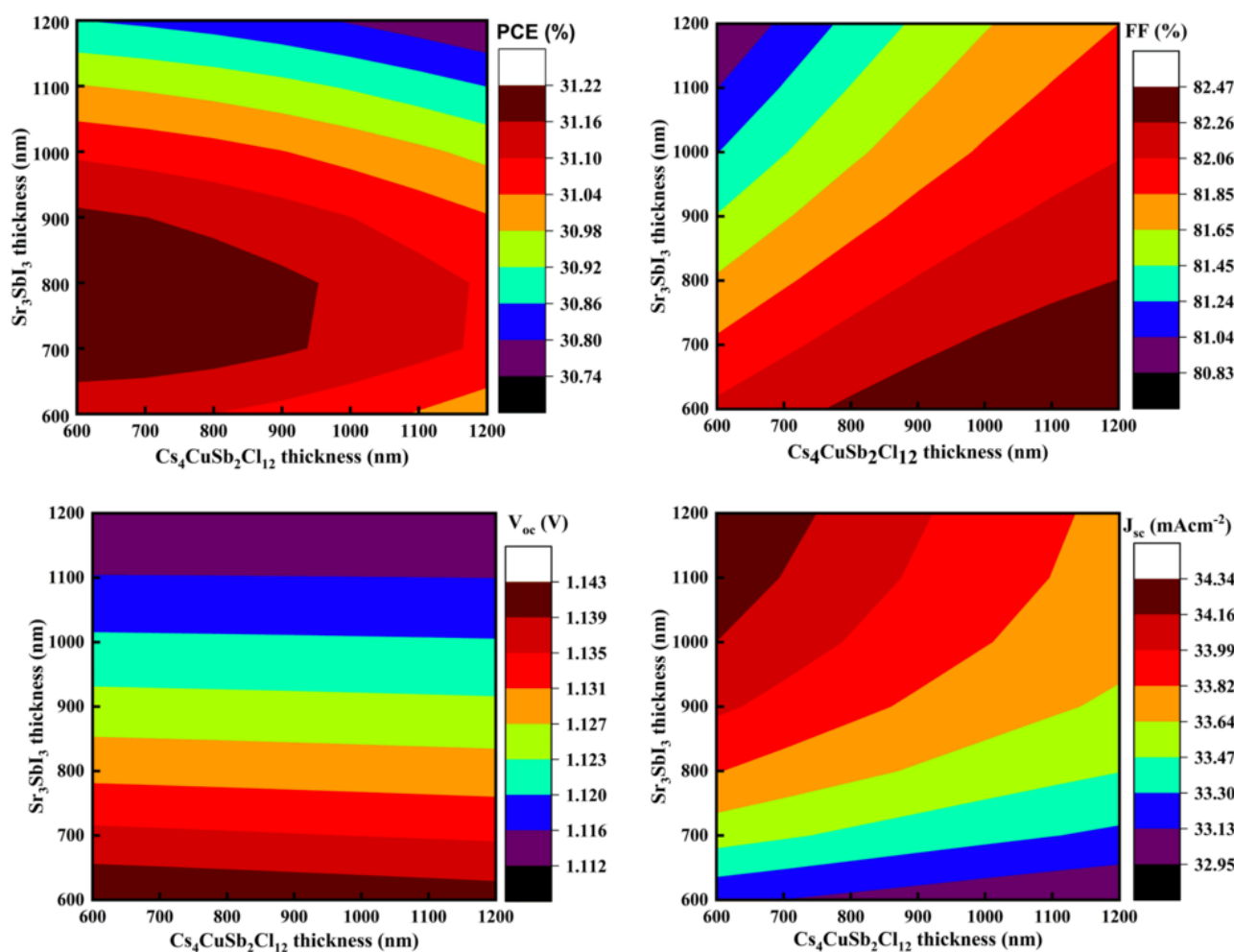


FIGURE 4: Modulation of device parameters with thickness variation of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ and Sr_3SbI_3 absorbing layers

PCE, power conversion efficiency; FF, fill factor

Similarly, V_{oc} and FF also decrease with increasing Sr_3SbI_3 thickness. This behavior can be attributed to enhanced bulk recombination arising from increased carrier transport length and trap-assisted recombination at higher absorber thicknesses. Although nanocrystals exhibit a direct bandgap, in this simulation the absorber is treated as an effective bulk layer with averaged optoelectronic parameters. Along with thickness optimization, doping also plays a significant role by improving charge carrier transport. Figure 5 shows that an increase in doping concentration of the n-type TiO_2 layer slightly increases the values of device parameters owing to reduced series resistance and improved charge extraction.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. *Cureus J Eng* 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

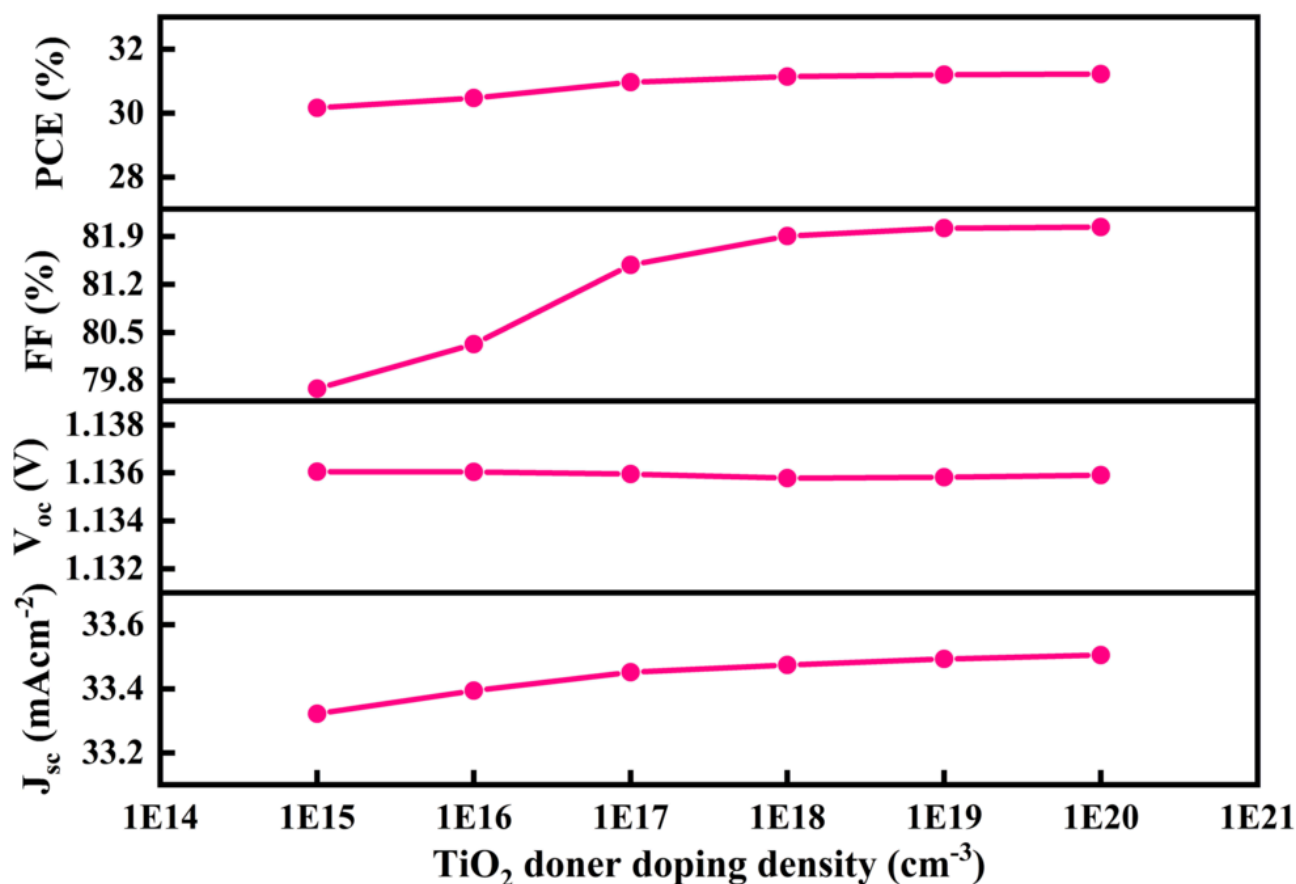


FIGURE 5: Device parameters variation with doping concentration of n-type TiO_2 layer

PCE, power conversion efficiency; FF, fill factor

However, further increase in doping concentration beyond $\sim 10^{19} \text{ cm}^{-3}$ saturates the device performance, which may be because the ETL is no more the limiting factor for device operation. The effect of bulk defect density in the absorber layers, which is inevitable in practical materials, is shown in Figure 6. The bulk defect density variation of the absorbing layers between 10^{11} and 10^{15} cm^{-3} causes the PCE to decrease with increasing defect density, from a maximum value of 35.22% at a defect concentration of 10^{11} cm^{-3} for both absorbers.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. *Cureus J Eng* 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

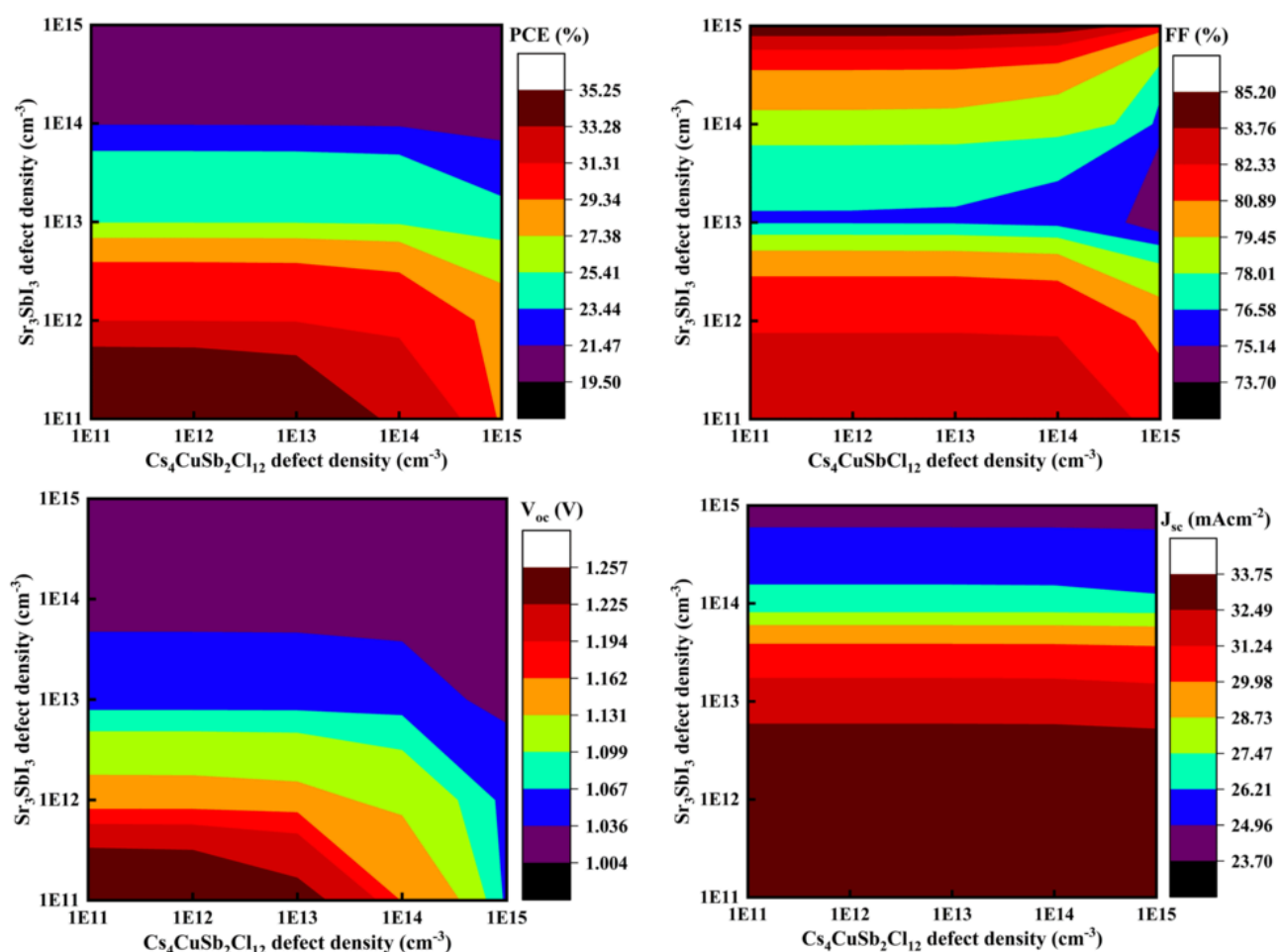


FIGURE 6: Device operational parameters variation with defect concentration of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ and Sr_3SbI_3 absorbing layers

PCE, power conversion efficiency; FF, fill factor

The PCE decline is due to the additional traps and shorter carrier lifetimes, resulting in enhanced bulk recombination. Experimentally reported defect densities typically lie in the range of $\sim 10^{14} \text{ cm}^{-3}$, corresponding to a simulated efficiency of 21.19%. Further, in order to fabricate intrinsically defect-free bulk perovskite layers, various techniques such as vapor phase processing, anti-solvent treatment, and others are analyzed. But, high-quality perovskite absorber layers with are yet to be fabricated experimentally. Still, the advanced vacuum film deposition techniques such as pulsed laser deposition, thermal evaporation, and RF sputtering may lead to the fabrication of low-defect-density perovskite films. Based on prior simulation studies, optimum defect densities of 10^{11} cm^{-3} and 10^{12} cm^{-3} were therefore selected for the $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ and Sr_3SbI_3 layers, respectively, to represent near-ideal absorber conditions, leading to a PCE of 31.28%. In addition to bulk defect densities, device operational parameters are also critically influenced by the imperfect interfaces between the subsequent layers. These heterointerfaces can introduce defect states that act as Shockley-Read-Hall recombination centers, enhancing non-radiative recombination and reducing carrier lifetime. Consequently, quasi-Fermi level splitting is suppressed leading to a decline in V_{oc} , and impeding charge extraction across the interface, thereby adversely affecting J_{sc} and fill factor. However, in this simulation interfacial defects are not extensively considered, as the analysis is primarily focused on investigating the intrinsic performance limits of the proposed double-layer architecture under optimistic conditions.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. *Cureus J Eng* 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

For further assessment, the device temperature was varied from 300 K to 380 K at an optimized absorber thickness of 700 nm for both the absorbing layers (Figure 7). An overall decline in device performance was observed with increasing temperature, except for the J_{sc} , which slightly increased due to the rise in intrinsic carrier concentration and saturation current at elevated temperatures.

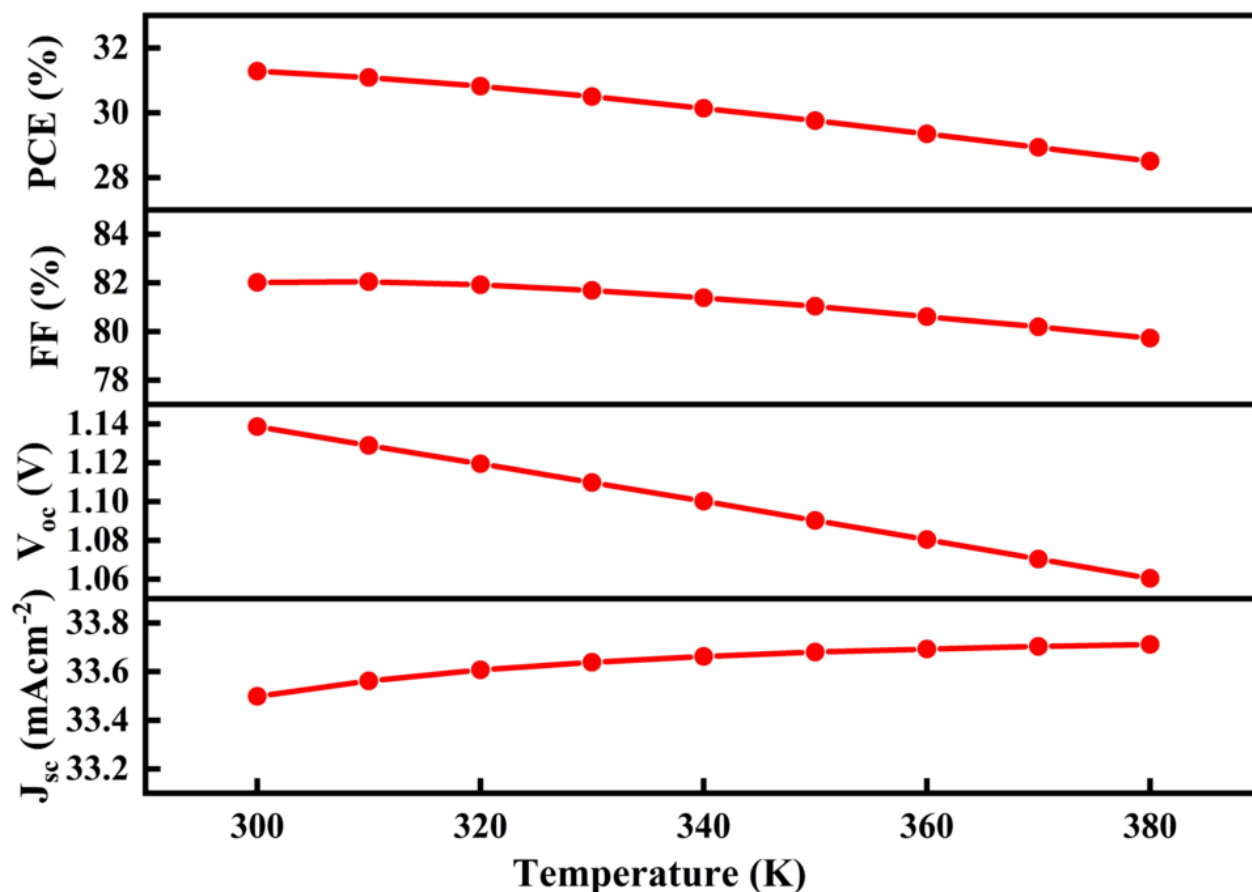


FIGURE 7: Variation in device parameters (PCE, FF, V_{OC} and J_{SC}) with temperature

PCE, power conversion efficiency; FF, fill factor

The reduction in V_{OC} and FF at higher temperatures is primarily associated with enhanced carrier recombination and increased thermal losses, which dominate over the marginal gain in saturation current. Figure 8 reflects the JV characteristics of the simulated devices adopting $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$, and $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ as active layers for single-layer and dual-layer architectures, respectively. The dual-absorber based device demonstrated a higher PCE of 35.22% owing to enhanced J_{sc} compared to the $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ based single-layer device, exhibiting a PCE of 30.11% under ideal defect density conditions. The gain in J_{sc} due to improved light absorption and carrier generation is enough to compensate for a slight reduction in V_{OC} and fill factor, which may be attributed to recombination and resistance losses due to the additional interface.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. *Cureus J Eng 3* : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

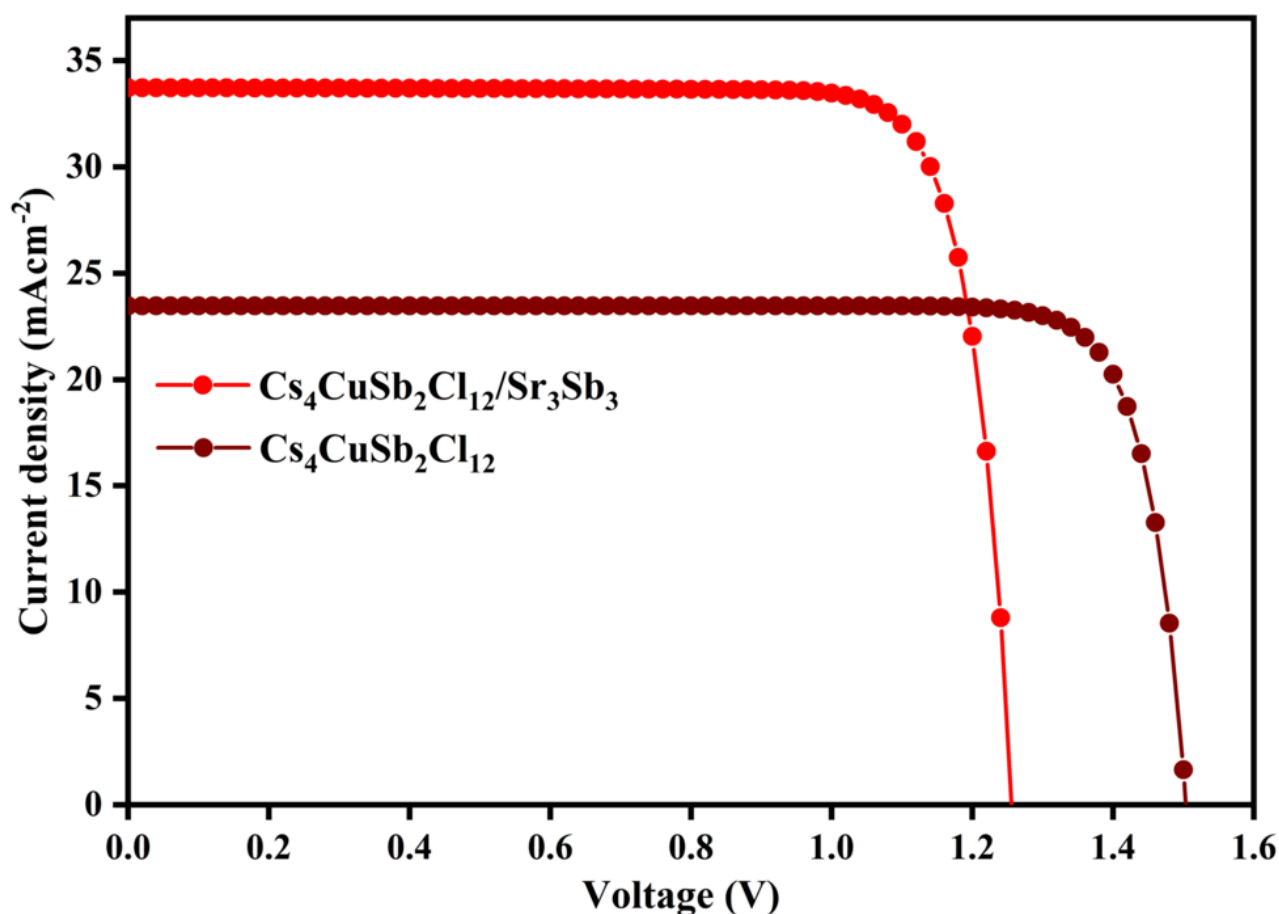


FIGURE 8: Current density-voltage characteristics of the optimized perovskite solar cell devices implementing $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$, and $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ as light absorber layers

Conclusions

In this work, the SCAPS-1D package was employed to assess the performance of PSCs based on dual absorbers $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ and Sr_3SbI_3 as active materials, which are non-toxic, long-term stable, and possess suitable direct band gaps. N-type TiO_2 and p-type Cu:NiO films were utilized as hole blocking and electron blocking layers, respectively. For optimized thickness (50 nm, 50 nm, 700 nm and 700 nm for TiO_2 , Cu:NiO , $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ and Sr_3SbI_3 layers respectively) and donor doping concentration of 10^{19} cm^{-3} for TiO_2 layer, the resulting device theoretically yielded a maximum PCE of 35.22% under idealized defect conditions (defect concentration of 10^{11} cm^{-3} for both $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ and Sr_3SbI_3 layers), which is considerably higher compared to the PCE of 30.11% obtained for $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ based device, owing to harvesting a broad range of solar spectrum. Also, a PCE of 21.19% was attained under realistic conditions (10^{14} cm^{-3} defect density for both the absorbing layers). Interfacial defects were not extensively considered in order to focus on upper-bound performance and isolate the effect of bulk material parameters; therefore, the reported results should be interpreted as near-ideal estimates. Furthermore, among all varied parameters, the absorber bulk defect density most strongly influenced device performance, as reduced trap states suppress bulk recombination, thus suggesting recombination control as a key factor for achieving high power output.

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. *Cureus J Eng 3* : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

Additional Information

Author Contributions

All authors have reviewed the final version to be published and agreed to be accountable for all aspects of the work.

Concept and design: Ritu Paliwal, Subhash C. Yadav, Yugal S. Kasana, Jagdish P. Yadav, Nidhi Agrawal, Dinesh K. Yadav, Balram Tripathi, Jitendra K. Mishra

Acquisition, analysis, or interpretation of data: Ritu Paliwal, Subhash C. Yadav, Dinesh K. Yadav, Balram Tripathi, Jitendra K. Mishra

Drafting of the manuscript: Ritu Paliwal, Subhash C. Yadav, Nidhi Agrawal

Critical review of the manuscript for important intellectual content: Ritu Paliwal, Subhash C. Yadav, Yugal S. Kasana, Jagdish P. Yadav, Dinesh K. Yadav, Balram Tripathi, Jitendra K. Mishra

Supervision: Jitendra K. Mishra

Disclosures

Human subjects: All authors have confirmed that this study did not involve human participants or tissue. **Animal subjects:** All authors have confirmed that this study did not involve animal subjects or tissue. **Conflicts of interest:** In compliance with the ICMJE uniform disclosure form, all authors declare the following: **Payment/services info:** All authors have declared that no financial support was received from any organization for the submitted work. **Financial relationships:** All authors have declared that they have no financial relationships at present or within the previous three years with any organizations that might have an interest in the submitted work. **Other relationships:** All authors have declared that there are no other relationships or activities that could appear to have influenced the submitted work.

Data Availability Statements

The datasets (and/or code) supporting this study are available from the corresponding author upon reasonable request.

Acknowledgements

Ritu Paliwal is thankful to CSIR-HRDG for awarding the "JRF Fellowship" (09/0149(19527)/2024-EMR-I). The authors would like to thank Mr. Marc Burgelman, of the Electronics and Information Systems (ELIS), Ghent University, Belgium, for providing free access to the SCAPS 1D simulation tool upon request.

References

1. Lim J, Park NG, Il Seok S, Saliba M: [All-perovskite tandem solar cells: from fundamentals to technological progress](#). Energy & Environmental Science. 2024, 17:4390-4425. [10.1039/d3ee03638c](#)
2. Jung HS, Park NG: [Perovskite solar cells: from materials to devices](#). Small. 2015, 11:10-25. [10.1002/smll.201402767](#)
3. Baikie T, Fang Y, Kadro JM, et al.: [Synthesis and crystal chemistry of the hybrid perovskite \(CH₃NH₃\)PbI₃ for solid-state sensitised solar cell applications](#). Journal of Materials Chemistry A. 2013, 1:5628-5641. [10.1039/c3ta10518k](#)
4. Song Y, Osheroov A, Bulović V, Kong J: [Graphene-perovskite Schottky barrier solar cells](#). Advanced Sustainable Systems. 2018, 2:1700106. [10.1002/adss.201700106](#)
5. Lee MM, Teuscher J, Miyasaka T, Murakami TN, Snaith HJ: [Efficient hybrid solar cells based on meso-superstructured organometal halide perovskites](#). Science. 2012, 338:643-647. [10.1126/science.1228604](#)
6. Yan J, Li H, Aldamasy MH, Frasca C, Abate A, Zhao K, Hu Y: [Advances in the synthesis of halide perovskite single crystals for optoelectronic applications](#). Chemistry of Materials. 2023, 35:2683-2712. [10.1021/acs.chemmater.2c03505](#)

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of Cs₄CuSb₂Cl₁₂/Sr₃SbI₃ Dual Absorber Lead-Free Perovskite Solar Cells. Cureus J Eng 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

7. Kusuma FJ, Widiyanto E, Wahyono W, et al.: [Optimizing novel device configurations for perovskite solar cells: Enhancing stability and efficiency through machine learning on a large dataset](#). Renewable Energy. 2025, 247:122947.
8. Liu X, Wu J, Zhang T, et al.: [Simultaneously mitigating anion and cation defects both in bulk and interface for high-effective perovskite solar cells](#). Solar RRL. 2022, 6:2100979. [10.1002/solr.202100979](#)
9. Xiao Z, Meng W, Wang J, Yan Y: [Thermodynamic stability and defect chemistry of bismuth-based lead-free double perovskites](#). ChemSusChem. 2016, 9:2628-2633. [10.1002/cssc.201600771](#)
10. Cai T, Shi W, Hwang S, et al.: [Lead-free \$\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}\$ layered double perovskite nanocrystals](#). Journal of the American Chemical Society. 2020, 142:11927-11936. [10.1021/jacs.0c04919](#)
11. Qi X, Zhang Y, Ou Q, et al.: [Photonics and optoelectronics of 2D metal-halide perovskites](#). Small. 2018, 14:e1800682. [10.1002/smll.201800682](#)
12. Sun S, Lu M, Gao X, Shi Z, Bai X, Yu WW, Zhang Y: [0D perovskites: unique properties, synthesis, and their applications](#). Advanced Science. 2021, 8:e2102689. [10.1002/adv.202102689](#)
13. Zhao D, Liang C, Wang B, et al.: [Overcoming the limitation of \$\text{Cs}_2\text{AgBiBr}_6\$ double perovskite solar cells through using mesoporous \$\text{TiO}_2\$ electron extraction layer](#). Energy & Environmental Materials. 2022, 5:1317-1322. [10.1002/eem2.12249](#)
14. Choudhary D, Kaur M, Sharma G, et al.: [Impact of halide variation on the optoelectronic properties of double perovskites](#). Scientific Reports. 2025, 15:33629. [10.1038/s41598-025-98686-6](#)
15. Yadav SC, Satrughna JAK, Shirage PM: [Investigation of the potential solar cell application of \$\text{Cs}_2\text{AgBiBr}_6\$ lead-free double perovskite](#). Journal of Physics and Chemistry of Solids. 2023, 181:111515. [10.1016/j.jpcs.2023.111515](#)
16. Yadav SC, Srivastava A, Manjunath V, Kanwade A, Devan RS, Shirage PM: [Properties, performance and multidimensional applications of stable lead-free \$\text{Cs}_2\text{AgBiBr}_6\$ double perovskite](#). Materials Today Physics. 2022, 26:100731. [10.1016/j.mtphys.2022.100731](#)
17. Singhal N, Chakraborty R, Ghosh P, Nag A: [Low-bandgap \$\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}\$ layered double perovskite: synthesis, reversible thermal changes, and magnetic interaction](#). Chemistry - An Asian Journal. 2018, 13:2085-2092. [10.1002/asia.201800635](#)
18. Vargas B, Ramos E, Pérez-Gutiérrez E, Alonso JC, Solís-Ibarra D: [A direct bandgap copper-antimony halide perovskite](#). Journal of the American Chemical Society. 2017, 139:9116-9119. [10.1021/jacs.7b04119](#)
19. Wang XD, Miao NH, Liao JF, et al.: [The top-down synthesis of single-layered \$\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}\$ halide perovskite nanocrystals for photoelectrochemical application](#). Nanoscale. 2019, 11:5180-5187. [10.1039/c9nr00375d](#)
20. Wang K, Jin Z, Liang L, et al.: [All-inorganic cesium lead iodide perovskite solar cells with stabilized efficiency beyond 15%](#). Nature Communications. 2018, 9:4544. [10.1038/s41467-018-06915-6](#)
21. Boukourt N, Patané S, Hadri B: [Development of high-efficiency PERC solar cells using Atlas Silvaco](#). Silicon. 2019, 11:145-152. [10.1007/s12633-018-9838-8](#)
22. Bhattarai S, Sharma A, Muchahary D, Gogoi D, Das TD: [Numerical simulation study for efficiency enhancement of doubly graded perovskite solar cell](#). Optical Materials. 2021, 118:111285. [10.1016/j.optmat.2021.111285](#)
23. Smucker J, Gong J: [A comparative study on the band diagrams and efficiencies of silicon and perovskite solar cells using wxAMPS and AMPS-1D](#). Solar Energy. 2021, 228:187-199. [10.1016/j.solener.2021.09.066](#)
24. Yang LM, Pan CY, Lu FP, Chang CW, Feng SW, Tu LW: [Anti-reflection sub-wavelength structures design for InGaN-based solar cells performed by the finite-difference-time-domain \(FDTD\) simulation method](#). Optics & Laser Technology. 2015, 67:72-77. [10.1016/j.optlastec.2014.09.016](#)
25. Alla M, Manjunath V, Chawki N, Singh D, Yadav SC, Rouchdi M, Boubker F: [Optimized \$\text{CH}_3\text{NH}_3\text{PbI}_3\text{-XCIX}\$ based perovskite solar cell with theoretical efficiency exceeding 30%](#). Optical Materials. 2022, 124:112044. [10.1016/j.optmat.2022.112044](#)
26. Yadav SC, Sharma A, Devan RS, Shirage PM: [Role of different counter electrodes on performance of \$\text{TiO}_2\$ based dye-sensitized solar cell \(DSSC\) fabricated with dye extracted from Hibiscus Sabdariffa as sensitizer](#). Optical Materials. 2022, 124:112066. [10.1016/j.optmat.2022.112066](#)
27. Feng M, Wang M, Zhou H, Li W, Wang SP, Zang Z, Chen S: [High-efficiency and stable inverted planar perovskite solar cells with pulsed laser deposited Cu-doped \$\text{NiO}_x\$ hole-transport layers](#). ACS Applied Materials & Interfaces. 2020, 12:50684-50691. [10.1021/acsami.0c15923](#)

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. Cureus J Eng 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>

28. Yadav SC, Manjunath V, Srivastava A, Devan RS, Shirage PM: [Stable lead-free \$\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}\$ layered double perovskite solar cells yielding theoretical efficiency close to 30%](#). Optical Materials. 2022, 132:112676. [10.1016/j.optmat.2022.112676](#)
29. Raj A, Kumar M, Kumar A, Laref A, Anshul A: [Investigating the potential of lead-free double perovskite \$\text{Cs}_2\text{AgBiBr}_6\$ material for solar cell applications: A theoretical study](#). International Journal of Energy Research. 2022, 46:13801-13819. [10.1002/er.8099](#)
30. Jayan KD: [Bandgap tuning and input parameter optimization for lead-free all-inorganic single, double, and ternary perovskite-based solar cells](#). Solar RRL. 2022, 6:2100971. [10.1002/solr.202100971](#)
31. Khanom MKM, Biswas SK: [Performance analysis of \$\text{Sr}_3\text{SbI}_3\$ -based perovskite solar cell using SCAPS-1D software](#). Advances in Materials Science and Engineering. 2025, 2025:11. [10.1155/amse/7134012](#)
32. Saha P, Singh S, Bhattacharya S: [Efficient and lead-free perovskite solar cells based on defect-ordered methyl ammonium antimony iodide](#). IEEE Transactions on Electron Devices. 2023, 70:1095-1101. [10.1109/ted.2023.3235870](#)

How to cite this article:

Paliwal R, Yadav S C, Kasana Y S, et al. (June 17, 2026) Theoretical Investigation and Device Modeling of $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{Sr}_3\text{SbI}_3$ Dual Absorber Lead-Free Perovskite Solar Cells. Cureus J Eng 3 : es44388-026-00124-4. DOI <https://doi.org/10.7759/s44388-026-00124-4>