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RESEARCH ARTICLE

High–Efficiency Lead~Free FAMASnGeI₃/ MASnBr₃ Perovskite Solar Cells: A Comprehensive Numerical Optimization Study Using SCAPS–1D

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ABSTRACT: Perovskite solar cells (PSCs) have emerged as a promising photovoltaic technology due to their high power conversion efficiency (PCE) and cost-effective fabrication. However, the toxicity of lead-based perovskites, such as MAPbI₃, poses significant environmental and health concerns, limiting their large-scale commercialization. This study explores lead-free alternatives by designing and simulating a double-absorber perovskite solar cell with the structure FTO/TiO₂/MASnBr₃/FAMASnGeI₃/NiO/Au using the SCAPS-1D simulation tool. The proposed device leverages the complementary bandgap properties of MASnBr₃ (1.3 eV) and FAMASnGeI₃ (1.4 eV) to enhance light absorption across the visible spectrum. A systematic optimization of key parameters—including layer thickness, doping concentration, and defect density—was conducted to maximize PCE. The optimal configuration features a 10 nm TiO₂ electron transport layer (ETL), a 150 nm MASnBr₃ absorber, a 225 nm FAMASnGeI₃ absorber, and a 150 nm NiO hole transport layer (HTL). Additionally, defect densities were minimized to 10¹³ cm⁻³ (MASnBr₃) and 10⁹ cm⁻³ (FAMASnGeI₃) to suppress non-radiative recombination. The optimized device achieved a record PCE of 34.70%, with an open-circuit voltage (Voc) of 1.3284 V, a short-circuit current density (Jsc) of 28.86 mA/cm², and a fill factor (FF) of 90.52%. Further analysis revealed that low series resistance (0 $\Omega \cdot cm^2$) and high shunt resistance (10⁷ $\Omega \cdot cm^2$) are critical for minimizing losses. This study provides a theoretical foundation for fabricating high-efficiency, environmentally friendly perovskite solar cells and highlights the potential of tin-based perovskites as viable alternatives to lead-based counterparts.

Keywords: Lead-free perovskite solar cells, FAMASnGeI₃/MASnBr₃, SCAPS-1D simulation, Defect density optimization, High-efficiency photovoltaics, Tin-based perovskites

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1. INTRODUCTION

Perovskite solar cells (PSCs) have emerged as one of the most promising photovoltaic technologies in recent years due to their exceptional power conversion efficiency (PCE), low-cost fabrication, and tunable optoelectronic properties [1, 2].

Lead-based perovskites, particularly methylammonium lead iodide (CH₃NH₃PbI₃), have dominated research efforts, achieving certified PCEs exceeding 25% [3–5]. However, the presence of toxic lead in these materials raises significant environmental and health concerns, hindering their largescale commercialization and deployment in consumer applications. The potential for lead leakage during manufacturing, operation, or disposal poses severe ecological risks, particularly in residential and agricultural settings. Consequently, the development of lead-free perovskite alternatives has become a critical research priority to ensure sustainable and environmentally benign photovoltaic technologies [6–9].

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Among the various lead-free perovskite candidates, tin (Sn)-based perovskites have garnered substantial attention due to their favorable optoelectronic properties and lower toxicity. Specifically, formamidinium-methylammonium tin germanium iodide (FAMASnGeI3) and methylammonium tin bromide (MASnBr3) exhibit narrow bandgaps of 1.4 eV and 1.3 eV, respectively, enabling broader absorption across the visible spectrum compared to CH₃NH₃PbI₃ (1.55 eV) [10–12]. This extended light-harvesting capability enhances charge carrier generation, making them promising candidates for high-efficiency solar cells. Additionally, the lower effective masses of electrons and holes in Sn-based perovskites facilitate superior charge transport properties, further improving device performance [13, 14]. Despite these advantages, Sn-based perovskites face challenges such as oxidation of Sn²⁺ to Sn⁴⁺, which introduces detrimental defects and accelerates charge recombination, ultimately limiting device efficiency and stability [15, 16]. Recent studies have explored compositional engineering, interfacial modifications, and defect passivation strategies to mitigate these issues, yet the full potential of FAMASnGeI3 and MASnBr3 remains underexplored, particularly in doubleabsorber perovskite solar cell configurations [17, 18].

This study addresses a critical research gap by presenting a comprehensive numerical investigation of a lead-free perovskite solar cell employing а FAMASnGeI₃/MASnBr₃ double-absorber architecture using the SCAPS-1D simulation platform. The novelty of this work lies in the systematic optimization of multiple device parameters, including layer thicknesses, doping concentrations, defect densities, and transport layer properties, to maximize photovoltaic performance. Unlike previous studies that focus on single-absorber configurations, this research explores the synergistic effects of combining (for broad-spectrum MASnBr₃ absorption) and FAMASnGeI₃ (for enhanced charge extraction), providing new insights into band alignment, carrier dynamics, and recombination suppression. Furthermore, this study introduces defect engineering strategies to minimize nonradiative losses, achieving a record simulated PCE of 34.70%, which represents a significant advancement in lead-free perovskite solar cell research.

The broader implications of this work extend beyond theoretical modeling, offering a practical roadmap for experimental fabrication of high-efficiency, environmentally sustainable PSCs. By elucidating the optimal device architecture and material parameters, this study contributes to the ongoing transition from lead-based to lead-free perovskite photovoltaics, aligning with global efforts toward green energy technologies. Future research directions include experimental validation, stability analysis under ambient conditions, and scalability assessments to facilitate realworld deployment. Ultimately, this work underscores the potential of FAMASnGeI₃/MASnBr₃-based PSCs as a viable alternative to conventional lead-based perovskites, paving the way for safer and more efficient solar energy solutions.

2. COMPUTATIONAL DETAILS

2.1. Simulation Methodology and Theoretical Framework

The numerical simulations presented in this study were conducted using the Solar Cell Capacitance Simulator (SCAPS-1D) version 3.3.10. well-established а computational tool that has been extensively validated for photovoltaic device modeling [10-13]. This simulation platform solves the fundamental set of coupled differential equations governing semiconductor device physics, including the Poisson equation for electrostatic potential distribution, and the continuity equations for electron and hole transport. The Poisson equation is expressed as $\nabla \cdot (\epsilon \nabla \psi)$ = - ρ , where ε represents the permittivity, ψ is the electrostatic potential, and p denotes the space charge density. The continuity equations account for carrier generation, recombination, and transport phenomena, incorporating both drift and diffusion components through the drift-diffusion model [14].

The simulation framework implemented in this work comprehensively models several critical physical processes that determine solar cell performance. These include optical absorption following the Beer-Lambert law, carrier generation profiles based on the incident AM1.5G solar spectrum, and multiple recombination mechanisms. The recombination models incorporated Shockley-Read-Hall (SRH) recombination through defect states in the bandgap, radiative recombination proportional to the product of electron and hole concentrations, and Auger recombination which becomes significant at high carrier densities. The defect physics were modeled using discrete energy levels within the bandgap, with capture cross-sections for electrons and holes specified for each defect type [15].

The numerical solution was obtained through finite difference methods with appropriate boundary conditions at each interface. Convergence criteria were rigorously enforced, requiring relative errors in potential and carrier concentrations to be below 10^{-6} between successive iterations. The simulation conditions replicated standard test conditions for photovoltaic devices, with an illumination intensity of 1000 W/m² under the AM1.5G spectrum and an operating temperature of 300 K, unless otherwise specified for temperature-dependent studies [16].

2.2. Device Architecture and Layer Specifications

The simulated device architecture, illustrated in Figure 1, consists of a six-layer heterostructure with the following configuration: FTO/TiO₂/MASnBr₃/FAMASnGeI₃/NiO/Au. Each layer was carefully parameterized based on experimental data and previous theoretical studies to ensure physical accuracy [17-20]. The fluorine-doped tin oxide (FTO) front contact was modeled with a thickness of 500 nm, electrical conductivity of 10⁴ S/cm, and optical transparency exceeding 80% across the visible spectrum. The titanium dioxide (TiO₂) electron transport layer (ETL) was

assigned a thickness of 10 nm, electron affinity of 4.2 eV, and doping concentration of 10^{17} cm⁻³ to ensure efficient electron extraction while maintaining adequate hole blocking capability.



Light Incident

Fig. 1. Schematic for the FTO/TiO₂/MASnBr₃/ FAMASnGe I₃/NiO/Au based solar cell.

The absorber layers consisted of methylammonium tin bromide (MASnBr₃) and formamidinium-methylammonium tin germanium iodide (FAMASnGeI₃) with thicknesses of 150 nm and 225 nm respectively. These materials were selected for their complementary bandgap energies (1.3 eV for MASnBr₃ and 1.4 eV for FAMASnGeI₃), enabling broad spectral absorption from 300 nm to 1000 nm. The nickel oxide (NiO) hole transport layer (HTL) was parameterized with a thickness of 150 nm, valence band maximum at 5.4 eV, and acceptor doping concentration of 3×10^{18} cm⁻³ to facilitate efficient hole collection. The gold back contact was modeled as an ideal ohmic contact with negligible contact resistance.

2.3. Material Parameters and Physical Models

The material parameters used in the simulations are summarized in Table 1, with values carefully selected from established literature sources [21-24]. Key electronic properties included bandgap energies (3.6 eV for NiO, 1.4 eV for FAMASnGeI₃, 1.3 eV for MASnBr₃, and 3.26 eV for TiO₂), electron affinities, and effective densities of states in the conduction and valence bands. Carrier mobilities were specified for each material, with particular attention given to the perovskite absorbers where electron and hole mobilities of 2 cm²/V·s and 1.6 cm²/V·s respectively were used based on reported values for tin-based perovskites [25].

Defect physics were modeled through bulk defect

2.4. Performance Evaluation and Optimization Methodology

The solar cell performance was evaluated through currentvoltage (J-V) characteristics under illumination, from which the key photovoltaic parameters were extracted: short-circuit current density (Jsc), open-circuit voltage (Voc), fill factor (FF), and power conversion efficiency (PCE). External quantum efficiency (EQE) spectra were calculated by monochromatic light simulation across the 300-1200 nm wavelength range. The initial simulation with baseline parameters yielded a PCE of 14.47% (Voc = 0.9171 V, Jsc = 32.74 mA/cm^2 , FF = 48.18%), which served as the reference for subsequent optimization studies [27].

The optimization procedure systematically varied key parameters including laver thicknesses. doping concentrations, and defect densities while monitoring their impact on device performance. Each parameter was varied within physically reasonable ranges: thicknesses from 10 nm to 1500 nm, doping concentrations from 10^{10} cm⁻³ to 10^{22} cm⁻³, and defect densities from 10^9 cm⁻³ to 10^{22} cm⁻³. Temperature-dependent studies covered the range from 250 K to 500 K to assess thermal stability. Series and shunt resistances were varied from 0 to 15 $\Omega \cdot cm^2$ and 10¹ to 10¹⁵ Ω ·cm² respectively to evaluate their impact on device performance [28]. The simulation methodology employed in this work provides a comprehensive framework for understanding and optimizing the performance of lead-free perovskite solar cells. By combining rigorous physical models with systematic parameter studies, this approach offers valuable insights for the experimental realization of high-efficiency, environmentally friendly photovoltaic devices.

3. RESULTS AND DISCUSSION

3.1. Optimization of thickness of TiO₂ (ETM) layer

The TiO₂ layer is essential in the solar cell as it is accountable for the charge transfer function and contributes to light transfer within the absorber layer. The variation of TiO₂ layer thickness, ranging from 10 nm to 500 nm, the simulated parameters are depicted in Figure 2. The results indicate that growing the thickness of the TiO₂ layer gives to a decay in the photovoltaic parameters. Consequently, the ETM layer thickness was reduced to 10 nm to attain improved PCE.

Table 1.	Initial	material	parameters for	r pro	posed	solar	cell used	in	SCAPS	Simulation.	
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Physical Parameters	Symbol	Unit	NiO (HTL)	FAMASnGeI3	MASnBr ₃	TiO ₂ (ETL)
Thickness	Th	nm	150	100	500	50
Energy Band Gap	Eg	eV	3.6	1.4	1.3	3.26
Electron Affinity	Х	eV	1.8	3.67	4.17	4.2
Dielectric Permittivity (Relative)	8 _r	-	11.7	8.2	10.0	10.0
Density of States at Valence Band	N_V	cm ⁻³	2.5X10 ²⁰	1.8X10 ¹⁹	1.8X10 ¹⁹	1.8X10 ¹⁸
Density of States at Conduction Band	N _C	cm ⁻³	2.5X10 ²⁰	2.2X10 ¹⁸	2.2X10 ¹⁸	2.2X10 ¹⁸
Thermal Velocity of Hole	Ve	cm/s	1X10 ⁷	1X10 ⁷	1X10 ⁷	1X10 ⁷
Thermal Velocity of electron	V_{h}	cm/s	1X10 ⁷	1X10 ⁷	1X10 ⁷	1X10 ⁷
Electron Mobility	μ _e	cm ² /V.s	2.8	2	1.6	20
Hole Mobility	$\mu_{\rm h}$	cm ² /V.s	2.8	2	1.6	10
Uniform Shallow Donor Doping	ND	cm ⁻³	0	1X10 ¹⁰	1X10 ¹³	1X10 ¹⁷
Uniform Shallow Acceptor Doping	NA	cm ⁻³	3X10 ¹⁸	1X10 ¹⁰	1X10 ¹³	0
Defect Density	N_t	cm ⁻³	1X10 ¹⁵	1.5X10 ¹⁵	1.5X10 ¹³	1X10 ¹⁵
References			[14]	[15]	[16]	[17]



Fig. 2. Effect of the thickness of ETM (TiO₂) on simulated parameters of solar cell.



Fig. 3. Variation of doping concentration of ETM (TiO₂) on the simulated parameters of solar cell.

The simulation at this optimal thickness of 10 nm shows an optimal performance parameters obtained are a Voc of 0.9198 V, a Jsc of 32.74 mA/cm^2 , an FF of 48.99%, and a PCE of 14.75%

3.2. Optimization of doping concentration of ETM layer (TiO₂)

Exploring the impact of varying doping concentration on the concert of the PSC involves adjusting the concentration of donor impurities (ND) in the value of 10⁹ to 10²¹ cm⁻³. As presented in Figure 3, increasing the doping concentration from 10⁹ to 10²¹ cm⁻³ results in an improvement in PCE, which rises from 14.74% to 14.95%. This enhancement in PCE is mainly recognised to a reduction in series resistance, which occurs owing to the increased optical conductivity of the ETM. Consequently, ND is optimized at 10²¹ cm⁻³ to achieve the best performance. Alongside the improvement in PCE, other photovoltaic parameters, such as Voc and FF, also show positive trends with increasing doping concentration. The optimized performance parameters at this doping concentration are as follows: PCE = 14.95%, Jsc = 32.74 mA/cm^2 , Voc = 0.9216 V, and FF = 49.55%. The improvement of these photovoltaic parameters with increasing ND can clarify by a reduction in the Auger recombination rate below a doping density of 10²¹ cm⁻³. Additionally, quenching losses are minimized when ND is kept below 10²¹ cm⁻³, contributing to the overall upgrading in the solar cell's performance.

3.3. Optimization of defect density (Nt) of ETM layer, TiO₂

The Nt in the ETL made of TiO2 plays an significant part in

determining the worth of the perovskite films and, consequently, the overall performance of perovskite solar cells. An increase in defect density within the perovskite layer can considerably reduce the solar cell's performance, as the optoelectronic properties are compromised due to electron or hole entrapment and recombination at defect sites within the bandgap. As the defect density rises from 10¹⁸ to 10²² cm⁻³, the PCE correspondingly decreases from 14.95% to 14.90%, as illustrated in Figure 4. This decrease in PCE is a direct consequence of the detrimental effects caused by higher defect levels, which disrupt the charge transport and increase recombination losses within the solar cell.

3.4. Optimization of thickness of Absorber layer, MASnBr₃

This layer is crucial for efficiency of solar cell as it is responsible for absorbing sunlight and generating electronhole pairs, which are important for energy conversion. Therefore, optimizing the thickness of the PAL is of paramount importance. Figure 5, demonstrations the variations in key photovoltaic parameters-Voc, Jsc, FF, and PCE—with respect to the MASnBr3 absorber layer thickness, which ranges from 25 to 1500 nm. As illustrated in Figure 5, the PCE gradually increases with the thickness of the layer MASnBr3 increases, reaching its peak efficiency of 19.88% when the layer is 150 nm thick. This increase in efficiency is due to enhanced absorption of light, which leads to greater generation of electron-hole pairs. However, beyond a thickness of 150 nm, the PCE begins to decline as the layer thickness of the absorber continues to increase. This reduction in efficiency attributed to an rise in electron-hole recombination within the layer, which outweighs the benefits of additional light absorption [18-21]. The Jsc value also exhibits a significant increase with the thickness of the

MASnBr₃ layer, rising sharply from 17.12 mA/cm² to 33.89 mA/cm² as the thickness rises from 25 nm to 1000 nm. This rise in Jsc is a result of improved light absorption, which enhances the generation of electron-hole pairs. Voc shows a declining tendency with increasing thickness, dropping from 1.04865 V to 0.8551 V. This decline in Voc is likely owing to a reduction in the effective bandgap and an increase in recombination losses, which negatively influence the Voc of the cell [22].

3.5. Optimization of donor density (ND) of MASnBr₃ layer

We examine the influence of modifying the concentration of Uniform Shallow Donors within the first absorber layer of MASnBr₃. We performed calculations of various photovoltaic parameters while adjusting the Uniform Shallow Donor concentration across a range from 10^{10} to 10^{22} cm⁻³ to determine the optimum value for this layer. The results, which include Voc, Jsc, FF, and PCE, are depicted in Figure 6. The figure illustrates how changes in the Uniform Shallow Donor concentration affect these photovoltaic parameters. As shown, varying the donor concentration impacts Voc, Jsc, and FF, culminating in the maximum PCE of approximately 23.66% at a Uniform Shallow Donor concentration of 5×10^{20} cm⁻³ within the MASnBr₃ absorber layer.



Fig. 4. Variation of the defect density of ETM (TiO₂) on simulated parameters of solar cell.



Fig. 5. Variation of the thickness MASnBr3 layer on simulated parameters of solar cell.



Fig. 6. Effect of the donor density (ND) of MASnBr3 layer on simulated parameters of solar cell.

3.6. Optimization of acceptor density (NA) of MASnBr3 layer

In this segment, we explore the influence of varying the concentration of Uniform Shallow Acceptors within the first absorber layer of MASnBr3. We conducted calculations of the photovoltaic parameters while adjusting the Uniform Shallow Acceptor concentration across a range from 10¹⁰ to 10²⁰ cm⁻³ to recognize the ideal value for the MASnBr₃ absorber layer in the proposed solar cell. The results, which include Voc, Jsc, FF, and PCE, shown in Figure 7. The figure shows that changes in the Uniform Shallow Acceptor concentration affect these photovoltaic parameters. Specifically, the highest PCE of approximately 24.70% attained at a Uniform Shallow Acceptor concentration of 1015 cm⁻³ within the absorber layer. This optimal concentration leads to improved Voc, Jsc, and FF, enhancing the overall efficiency of the proposed solar cell.



Fig. 7. Effect of the acceptor density (NA) of MASnBr3 layer on simulated parameters of solar cell.

3.7. Optimization of defect density (Nt) of Absorber layer, MASnBr₃

This layer is critical for essential functions such as carrier generation, carrier recombination, and charge transport. Thus, the feature of the absorber material shows a vibrant role in determining the solar cell's performance [23]. The defect density in perovskite materials, which refers to the amount of defects or impurities within the material, significantly influences solar cell characteristics. Defects in perovskites can include vacancies, interstitials, Frenkel defects, and Schottky defects [24-25]. These defects can poorly affect the optical, electrical, and thermal properties of the perovskite material, leading to deviations in the performance and solar cell efficiency. The occurrence of such defects can upset the generation and transport of charge carriers, increase recombination rates, and alter the material's overall stability, all of which add to the solar cell final efficiency. [23] The initial defect density (Nt) in the absorber layer is set at 10^{13} cm⁻³. Figure 8 displays the variation between photovoltaic (PV) parameters and Nt within the absorber layer. As

depicted, significant improvements in the photovoltaic parameters of the PSC are observed as Nt decreases, supporting with outcomes from studies on lead perovskites. At a Nt of 1.0×10^{13} cm⁻³, the cell demonstrates notable enhancements in performance, achieving a Jsc of 25.81 mA/cm², an Voc of 1.0646 V, a FF of 87.47%, and a PCE of 24.03%. The optimal Nt of 1.0×10^{13} cm⁻³ is selected because it maximizes all key PV parameters, reflecting the performance of the highest efficiency.

1.08 30 (a) 1.06 25 1.04 JSC (mA.cm () 00 1.02 voc 1 ISC 0.98 0.96 n 1.E+09 1.E+11 1.E+13 1.E+15 1.E+17 1.E+19 Defect Density (cm⁻³) 87.5 30 (b) 87.4 25 87.3 20 15 (%) FF (%) 87.2 87.1 10 87 5 86.9 1.E+11 1.E+13 1.E+15 1.E+17 1.E+19 1.E+09 Defect Density (cm⁻³)



3.8. Optimization of thickness of second Absorber layer, FAMASnGeI₃

Figure 9 displays the variants in Voc, Jsc, FF, and PCE as a function of FAMASnGeI₃ thickness, ranging from 25 to 1500 nm. The layer thickness of the FAMASnGeI₃ increases, the PCE rises steadily until it reaches its peak value of 24.64% at a thickness of 225 nm. Beyond this point, the PCE begins to decline with further increases in thickness. This decrease in PCE is due to increased electron-hole recombination within the absorption layer, rather than an increase in the generation

of electron-hole pairs. The Jsc value increases with the thickness of FAMASnGeI₃, rising from 23.50 mA/cm² to 24.64 mA/cm² over the thickness range of 25–1500 nm. This increase credited to improved light absorption. The Voc shows a slight decrease from 1.1608 V to 0.9671 V, which can be owing to a reduction in the effective bandgap and increased recombination losses.



Fig. 9. Variation of the thickness of Absorber layer FAMASnGeI₃ on simulated parameters of solar cell.

3.9. Optimization of donor density of second Absorber layer FAMASnGeI₃

In this section, we investigate the influence of varying the concentration of Uniform Shallow Donors within the second absorber layer of FAMASnGeI₃. Our analysis involves adjusting the donor concentration within the range of 10⁹ to 10²² cm⁻³ to identify the optimal value for the FAMASnGeI₃ layer in the planned solar cell. The results, including Voc, Jsc, FF and PCE presented in Figure 10. The figure demonstrates that changing the Uniform Shallow Donor concentration impacts these photovoltaic parameters. The highest PCE of approximately 25.73% is achieved at a Uniform Shallow

1.4

Donor concentration of 10¹⁹ cm⁻³ within the second absorber layer. This concentration provides the optimal balance, enhancing Voc, Jsc, and FF, and leading to the maximum efficiency for the solar cell.

This concentration optimizes Voc, Jsc, and FF, subsequent in the maximum efficiency.

29.5



Fig. 10. Variation of the simulated parameters with the donor density of Absorber layer FAMASnGeI₃.

3.10. Optimization of acceptor density of second Absorber layer FAMASnGeI₃

In this segment, we investigate the influence of varying the concentration of Uniform Shallow Acceptors within the second absorber layer of FAMASnGeI₃. The analysis involves calculating photovoltaic parameters while adjusting the Uniform Shallow Acceptor concentration from 10⁹ to 10²² cm⁻³ to determine the optimal value for the FAMASnGeI₃ layer in the planned solar cell. The results, including Voc, Jsc, FF, and PCE, are presented in Figure 11. The figure illustrates that changing the Uniform Shallow Acceptor concentration affects these photovoltaic parameters. The highest PCE of approximately 34.28% is achieved at a Uniform Shallow Acceptor concentration of 10²² cm⁻³ within the absorber layer.

29 1.2 28.5 (a) 1 28 SC () 0.8 000 0.6 27.5 VOC 27 JSC 26.5 0.4 26 0.2 25.5 0 25 1.00E+09 Doping concentration (cm⁻³) 91 40 90 35 89 30 (b) 88 25 (%) 87 20 는 86 15 PCF 85 10 84 5 83 0 1.00E+09 Doping concentration (cm⁻³)

Fig. 11. Effect of the simulated parameters with the acceptor density of Absorber layer FAMASnGeI₃.

3.11. Optimization of defect density of second Absorber layer FAMASnGeI₃

The initial defect density (Nt) within the second absorber layer is set at 10^{15} cm⁻³. Figure 12 shows the correlation between photovoltaic parameters and Nt within this layer. Significant improvements in the PV parameters of the PSC are observed as Nt decreases, consistent with similar studies on lead perovskites. At a defect density of 1.0×10^9 cm⁻³, the PV properties of the cell are notably enhanced, achieving a Jsc of 28.86 mA/cm², an Voc of 1.3284 V, a FF of 90.52%, and a PCE of 34.70%. The optimized defect density of 1.0×10^9 cm⁻³ is selected because it maximizes all key PV parameters, reflecting the highest efficiency of the cell.



Fig. 12. Effect of the simulated parameters with the defect density of absorber layer FAMASnGeI₃

3.12. Optimization of thickness of HTM layer (NiO)

The PCE of PSCs is significantly influenced by the ETL and HTL materials characteristics. Additionally, the thickness of these thin films is closely related to their electrical properties, which affect the transport of electrons & holes and directly impact the PCE. As presented in Figure 13, our investigation examines the effects of varving the thickness of the NiO HTL layer on the photovoltaic parameters, including Voc, Jsc, FF, and PCE. Extremely thin HTL films may develop micropinholes, which can generate direct contact between the absorber layer and the rear electrode, potentially compromising cell performance. Conversely, excessively thick HTL layers may increase the series resistance (Rs) at the boundary between the metal electrode and the HTL, adversely affecting the efficiency of the cell. The optimal HTL thickness balances these issues to enhance the performance of the PSC. [26]

As illustrated in Figure 13, the PCE of the PSCs shows no change with increasing HTL thickness at the initial acceptor density specified in Table 1. Figure 13 details the effects of varying HTL thickness on key performance parameters such as Voc, Jsc, FF, and PCE, with thickness ranging from 10 to 500 nm. The observed trends indicate that the optimal HTL thickness is 150 nm, as the PCE values stabilize beyond this thickness. This proposes that advance increases in HTL thickness do not contribute to significant improvements in efficiency, confirming 150 nm as the optimal thickness for maintaining consistent PCE values.



Fig. 13. Variation of the simulated parameters with the thickness of HTM (NiO).

3.13. Optimization of doping concentration of HTM layer (NiO)

Exploring the impact of varying the doping concentration of acceptor impurities (NA) on PSC performance involves adjusting the concentration within the range of 10^{10} to 10^{22} cm⁻³. As shown in Figure 14, changes in the doping concentration from 10^{10} to 10^{22} cm⁻³ do not significantly affect the performance of the PSC. The performance parameters, including PCE, Jsc, Voc, and FF, remain consistent across this range. The optimized performance

parameters observed are a PCE of 34.70%, Jsc of 28.86 mA/cm², Voc of 1.3284 V, and FF of 90.50%. Consequently, an acceptor impurity concentration (NA) of 10^{15} cm⁻³ is chosen for further calculations, as it provides the optimal performance while ensuring stable results across the doping range.



Fig. 14. Variation of the simulated parameters with the doping concentration of HTM (NiO).

3.14. Optimization of defect density of HTM layer (NiO)

The defect density of a Hole Transport Material (HTM) like NiO can significantly influence the superiority of perovskite films. An increase in defect density within the perovskite can substantially degrade the performance of the perovskite-based solar cells. This degradation occurs because defects lead to hole entrapment and increased recombination, which disrupts the optoelectronic properties of the material. As depicted in Figure 15, variations in defect density from 10¹⁰ to 10²² cm⁻³ do not significantly alter the performance of the perovskite-based solar cells within this configuration. This proposes that, regardless of changes in defect density, the solar cell performance remains relatively stable in this range.



Fig. 15. Variation of the simulated parameters with the defect density of HTM (NiO).

3.15. Effect of temperature

Understanding how temperature affects solar cell performance is crucial for determining the stability and solar cell efficiency. To investigate this, we change the operating temperature of the simulated model from 300 K to 500 K. As shown in Figure 16, temperature has a significant adverse impact on solar cell performance. As the temperature increases, the PCE decreases from 34.70% at 300 K to 31.32% at 500 K. This decline in efficiency with rising temperature is primarily due to a reduction in the diffusion length of charge carriers. Higher temperatures increase deformation stress on the layers, leading to more interfacial defects and poor interconnectivity between the layers. This poor interconnectivity results in an increased recombination rate in the absorber layer, further reducing the diffusion length and increasing series resistance. Consequently, these factors contribute to a decrease in cell performance. Therefore, the best performance of the proposed model is achieved at an operating temperature of 300 K.



Fig. 16. Variation of the simulated parameters with the temperature.

3.16. Effect of series resistance

In PSCs, sheet resistance originates from several internal sources, including internal resistances, interface barriers, charge-collecting interlayers, and metal-based electrodes. In contrast, shunt resistance (Rs) arises from leakage pathways such as recombination losses and pinholes within the photoactive layer. As the series resistance of a solar cell increases, the Jsc tends to decline progressively. This is because higher series resistance impedes the flow of current through the cell, leading to a reduction in Jsc. The Voc remains relatively unaffected by Rs, as the total current flow through the cell and the associated series resistance are minimal. Consequently, the PCE of a solar cell is typically lower when its series resistance is high; due to the decrease in short-circuit current while Voc remains stable [27-28]. To analyse the influence of series resistance (Rs) on the performance of PSCs, we investigated variations in Rs ranging from 0 to 15 $\Omega \cdot \text{cm}^2$. As presented in Figure 17, the PCE of the perovskite device structures decreased notably with increasing Rs, dropping from 34.70% to 23.03%. The FF also decreased as Rs increased. In contrast, the Jsc



Fig. 17. Effect of the simulated parameters with the series resistance.

3.17. Effect of shunt resistance

Figure 18 illustrates the impact of varying shunt resistance (Rsh) on the cell performance of the structures proposed, with Rsh ranging from 10^1 to $10^{15} \Omega \cdot \text{cm}^2$. As depicted, the Voc, PCE, and FF exhibit a rapid increase from 10^1 to $10^7 \Omega \cdot \text{cm}^2$, after which they stabilize and remain constant with additional increases in Rsh. In contrast, the Jsc remains constant across all shunt resistance values. The observed improvement in device efficiency is primarily recognised to the increase in FF. The optimized shunt resistance value, which maximizes device performance, was found to be $10^7 \Omega \cdot \text{cm}^2$ for the proposed perovskite solar cells.



Fig. 18. Effect of the simulated parameters with the shunt resistance.

4. CONCLUSION

This study presents a comprehensive numerical investigation of a lead-free perovskite solar cell (PSC) utilizing a FAMASnGeI₃/MASnBr₃ double-absorber structure simulated via SCAPS-1D. Through systematic optimization of layer thicknesses, doping concentrations, and defect densities, the proposed device achieved a record power conversion efficiency (PCE) of 34.70%, demonstrating the viability of tin-based perovskites as sustainable alternatives to toxic lead-based counterparts. The optimal thicknesses for the absorber layers were determined to be 150 nm for MASnBr3 and 225 nm for FAMASnGeI3, balancing light absorption and charge recombination. The electron transport layer (TiO₂) and hole transport layer (NiO) were optimized at 10 nm and 150 nm, respectively, ensuring efficient charge extraction. Doping concentrations were fine-tuned, with 10²¹ cm⁻³ for TiO₂ (ETL), 10¹⁵ cm⁻³ for MASnBr₃, and 10²² cm⁻³ for FAMASnGeI3, enhancing carrier mobility and reducing resistive losses. Defect density played a crucial role in

performance, where minimizing defects to 1013 cm⁻³ (MASnBr₃) and 10⁹ cm⁻³ (FAMASnGeI₃) significantly improved Voc (1.3284 V) and FF (90.52%) by suppressing Shockley-Read-Hall recombination. Additionally, temperature-dependent simulations revealed that 300 K is the optimal operating condition, with efficiency declining at higher temperatures due to increased charge recombination. The study also highlighted the importance of low series resistance (0 $\Omega \cdot cm^2$) and high shunt resistance (10⁷ $\Omega \cdot cm^2$) in maximizing PCE. These findings provide critical insights for experimentalists aiming to fabricate high-performance, lead-free PSCs. Future work should focus on experimental validation, stability analysis, and interface engineering to further enhance efficiency and scalability.

DECLARATIONS

Ethical Approval

We affirm that this manuscript is an original work, has not been previously published, and is not currently under consideration for publication in any other journal or conference proceedings. All authors have reviewed and approved the manuscript, and the order of authorship has been mutually agreed upon.

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Availability of data and material

The datasets generated and/or analyzed during the current study are available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare that they have no financial or personal interests that could have influenced the research and findings presented in this paper. The authors alone are responsible for the content and writing of this article.

Authors' contributions

All authors contributed equally to this work.

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