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Abstract

Cesium-formamidinium-methylammonium lead iodide-bromide (CsFAMAPbIBr) perovskite has gained attentions because its combine high efficiency potential with improved compositional stability. Carbon electrodes provide a low-cost alternative to noble-metal contacts in perovskite solar cells (PSCs), and can be applied using simple printing techniques. This study employs SCAPS-1D to systematically optimize an FTO/BaSnO₃/CsFAMAPbIBr/Cu₂O/C solar cell while retaining a carbon back electrode and experimentally attainable input parameters. The prototype device exhibited a power conversion efficiency (PCE) of 19.91%, with V_{OC} , J_{SC} and FF of 1.24 V, 21.47 mA/cm², and 74.79%, respectively. Systematic variation of layer thickness, carrier concentration, bulk and interface defect densities, and series and shunt resistances increased the PCE to 26.97%, with V_{OC} , J_{SC} and FF of 1.32 V, 23.90 mA/cm², and 85.23%, respectively. Sensitivity evaluation identified absorber bulk defect density and shunt resistance as the major performance-limiting parameters, with sensitivities of 0.713 and 0.515, respectively. Temperature-dependent simulations showed a consistent PCE above 26% between 290 and 330 K. These results establish practical design priorities for efficient carbon-electrode triple-cation mixed-halide PSCs

and provide an experimentally oriented strategy for translating numerical optimization toward device fabrication.

1. Introduction

Perovskite solar cells (PSCs) have emerged as favourable next-generation photovoltaic devices because of their remarkable strong optical absorption, adjustable bandgap, extended charge-carrier diffusion length, low exciton-binding energy, and suitability for low-temperature solution-based fabrication. [1-3]. Among the different absorber compositions, triple-cation mixed-halide perovskites containing Cs^+ , FA^+ and MA^+ with I^-/Br^- have attracted particular attention because compositional engineering improves phase stability while retaining favourable optical and charge-transport properties. Cesium-formamidinium-methylammonium lead iodide-bromide (CsFAMAPbIBr) compositions such as $\text{Cs}_{0.05}\text{FA}_{0.79}\text{MA}_{0.15}\text{PbI}_{2.45}\text{Br}_{0.55}$ provide an attractive balance between efficiency and stability for high-performance PSCs [4-6].

Considerable experimental progress has already been made with CsFAMAPbIBr absorbers. Wu et al. (2017) obtained a PCE of 19.61% through solvent engineering of dense and pinhole-free triple-cation films [7], while Jung and Lee (2021) achieved 16.01% by controlling the reaction time during ambient-air sequential deposition [8]. Lee et al. (2021) subsequently increased the PCE to 19.70% using dynamic spin coating [8]. More recently, Park et al. (2025) achieved 20.01% by gamma-ray modification of the SnO_2 electron-selective layer (ETL) [9]. Despite these advances, most experimentally demonstrated CsFAMAPbIBr PSCs employ Spiro-OMeTAD together with an evaporated Au rear electrode. The dependence on costly noble metals and vacuum deposition partly offsets the low-cost manufacturing advantage expected from perovskite photovoltaics.

Numerical modelling has also been extensively used to optimize CsFAMAPbIBr PSCs. Alanazi and Eid (2023) simulated $\text{ITO}/\text{SnO}_2/\text{Cs}_{0.05}\text{FA}_{0.79}\text{MA}_{0.15}\text{PbI}_{2.45}\text{Br}_{0.55}/\text{Spiro-OMeTAD}/\text{Au}$ and obtained PCEs of 22.16% [5], while demonstrating the importance of interface defects, absorber thickness and band alignment. Saidani et al. (2025) reported 28.01% for an Ag-contacted CsFAMAPbIBr cell [10], whereas Elmourabit et al. (2025) predicted 34.75% using an Au rear electrode in the configuration $\text{FTO}/\text{PCBM}/\text{Cs}_{0.05}(\text{MA}_{0.17}\text{FA}_{0.83})_{0.95}\text{Pb}(\text{I}_{0.83}\text{Br}_{0.17})_3$

/MeO–2PACz/Au [11]. However, the latter model idealized series and shunt resistances, which are unavoidable sources of loss in practical PSCs. Thus, very high simulated efficiencies may represent theoretical device potential without necessarily providing experimentally accessible fabrication conditions.

The rear electrode is an important unresolved issue. Au and Ag offer favourable conductivity and contact energetics but increase material and processing costs. Carbon provides a more attractive alternative because it is abundant, inexpensive, chemically stable and compatible with scalable printing techniques [12]. A recent CsFAMAPbIBr simulation by Jubu et al. (2026) considered carbon in the prototype device; however, carbon was subsequently replaced by Au in the optimized architecture to obtain a high PCE of 29.08% [13]. This leaves an important practical gap: can a competitive CsFAMAPbIBr PSC be optimized while retaining carbon as the final rear electrode rather than replacing it with a noble metal solely to maximize simulated efficiency?

A second limitation of many numerical PSC studies is the use of highly idealized parameter combinations that may be difficult to reproduce experimentally. The present work therefore adopts a different optimization approach. Rather than seeking the highest mathematically achievable PCE, the simulation parameters are restricted to experimentally defensible ranges. The carrier concentrations of BaSnO₃ and Cu₂O are selected from experimentally reported ranges [14-17], while the CsFAMAPbIBr carrier concentration is supported by experimental studies [18, 19]. The optimized BaSnO₃, CsFAMAPbIBr and Cu₂O thicknesses are similarly constrained by experimentally attainable film dimensions reported in the literature.

Practical electrical and defect-related losses are also retained rather than removed during optimization. The adopted bulk defect densities are supported by experimental reports [21, 21], while the minimum interface defect densities are consistent with experimentally passivated PSC interfaces [22, 23]. Likewise, finite series and shunt resistances are included using experimentally supported values [19, 24, 25]. This approach avoids obtaining an artificially high efficiency through simultaneous assumptions of negligible resistance, defect-free interfaces, unrealistic doping levels and ideal contact conditions.

This study investigates the FTO/BaSnO₃/Cs_{0.05}FA_{0.79}MA_{0.15}PbI_{2.45}Br_{0.55}/Cu₂O/C architecture using SCAPS-1D, with emphasis on experimentally realizable optimization. The effects of transport-layer selection, layer thickness, carrier concentration, bulk and interface defect

densities, absorber bandgap, series and shunt resistance, and back-contact work function are systematically examined. The optimized carbon-contact device achieves a competitive PCE. It is hoped that this study would contribute to the body of knowledge on CsFAMAPbIBr-based PSCs.

2.0 Numerical Simulation

SCAPS-1D employs a physics-based numerical framework to describe the coupled optical and electrical behaviour of multilayer thin-film photovoltaic devices. In this study, the program was adopted because it provides an efficient platform for analysing carrier generation and transport, recombination losses, defect states, energy-band alignment, and interfacial processes within perovskite solar cells. The device response is obtained by self-consistently solving Poisson's equation (Eq. 1) together with the electron and hole continuity equations (Eqs. 2 and 3). Its ability to systematically vary bulk and interface defects, transport-layer properties, contact conditions, and AC-response parameters makes SCAPS-1D particularly useful for identifying performance-limiting mechanisms and optimizing PSC architectures [26, 27].

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

$$\frac{1}{q} \left(\frac{dJ_n}{dx} \right) = G(x) - R(x) \quad 2$$

$$-\frac{1}{q} \left(\frac{dJ_p}{dx} \right) = G(x) - R(x) \quad 3$$

where ψ represents the electrostatic potential, ε denotes permittivity, q represents magnitude of the charge of an electron, and n , p , n_t , and p_t symbolize the free electron, free hole, trapped electron, and trapped hole, respectively. N_A^- stand for the ionized acceptor-like doping concentration, and N_D^+ designates the ionized donor-like doping concentration and. J_p and J_n designate the hole and electron current densities, respectively. $R(x)$ is the total recombination rate, and G_{op} denotes the optical generation rate. The recombination through deep traps inside the energy gap is described by Shockley Read Hall (SRH) recombination model [3]. The SRH recombination bulk defects are characterized by bulk electron and hole lifetimes (τ_n and τ_p). Moreover, the interface recombination

can be described between two adjacent layers. This interfacial recombination is explained by the Pauwels-Vanhoutte theory [28], where thermionic emission assumes its implementation.

The relations for the electron and hole quasi- Fermi levels (E_{Fn} , and E_{Fp}) for the electron and hole current densities are described by Eqs. 4 and 5.

$$J_n = q\mu_n n \frac{dE_{Fn}}{dx} \quad 4$$

$$J_p = q\mu_p p \frac{dE_{Fp}}{dx} \quad 5$$

where μ_p and μ_n are the hole and electron mobility, respectively.

For deep-level defects, the Shockley-Read-Hall recombination rate can be written according Eq. 6, where n_1 and p_1 are given by Eqs. 7 & 8, and the carrier lifetimes associated with the defect population can be expressed by Eq. 9.

$$R_{SRH} = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \quad 6$$

$$n_1 = N_c \exp\left(\frac{E_c - E_t}{k_B T}\right) \quad 7$$

$$p_1 = N_v \exp\left(-\frac{E_t - E_v}{k_B T}\right) \quad 8$$

$$\tau_n = \frac{1}{\sigma_n v_{th} N_t}, \quad \tau_p = \frac{1}{\sigma_p v_{th} N_t} \quad 9$$

where τ_n is electron lifetime, τ_p is hole lifetime (s), σ_n is electron capture cross-section of the defect σ_p is hole capture cross-section of the defect state, v_{th} is thermal velocity of the charge carriers, and N_t is defect or trap density in the semiconductor.

2.1 Device structure and rationale

A carbon-electrode-based PSC architecture was designed in the form FTO/ETL/CsFAMAPbIBr/HTL/C, where BaSnO₃, IGZO, SnS₂, PCMB, and TiO₂ were

considered as alternative electron transport layers, while Cu_2O , CuO , PEDOT:PSS, P3HT, and V_2O_5 were evaluated as hole transport layers. The schematic configuration of the device is presented in Fig. 1a. In this multilayer heterojunction structure, incident light enters through the transparent FTO front contact and reaches the CsFAMAPbI₃ absorber, where photogenerated charge carriers are produced. The ETL is responsible for selective electron extraction and transport, supported by its suitable bandgap, electron affinity, and carrier-transport properties. Conversely, the HTL promotes hole extraction toward the rear electrode while limiting recombination at the interface and undesirable electron transfer at the back contact. A carbon work function of 5.0 eV was adopted for the rear electrode [13]. The corresponding energy-level alignment of the investigated ETLs and HTLs is illustrated in Fig.

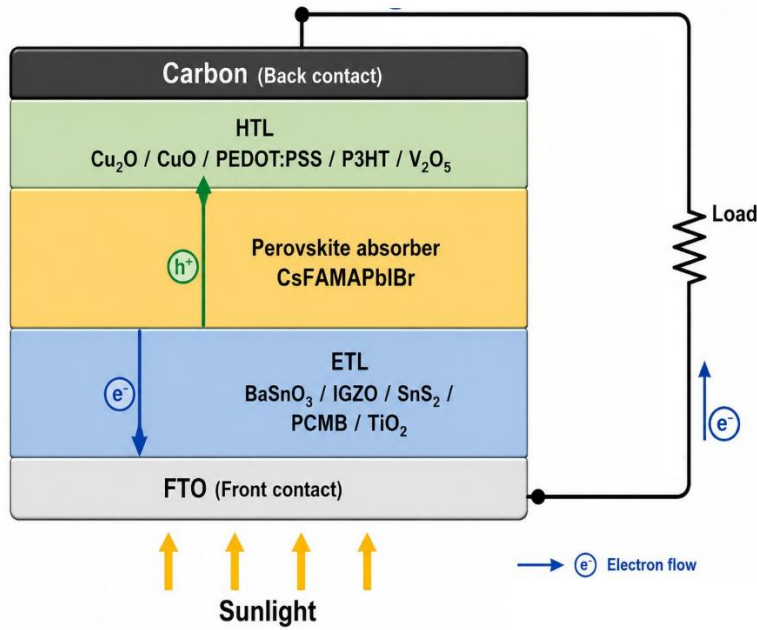


Fig. 1. Schematic of the PSC architecture.

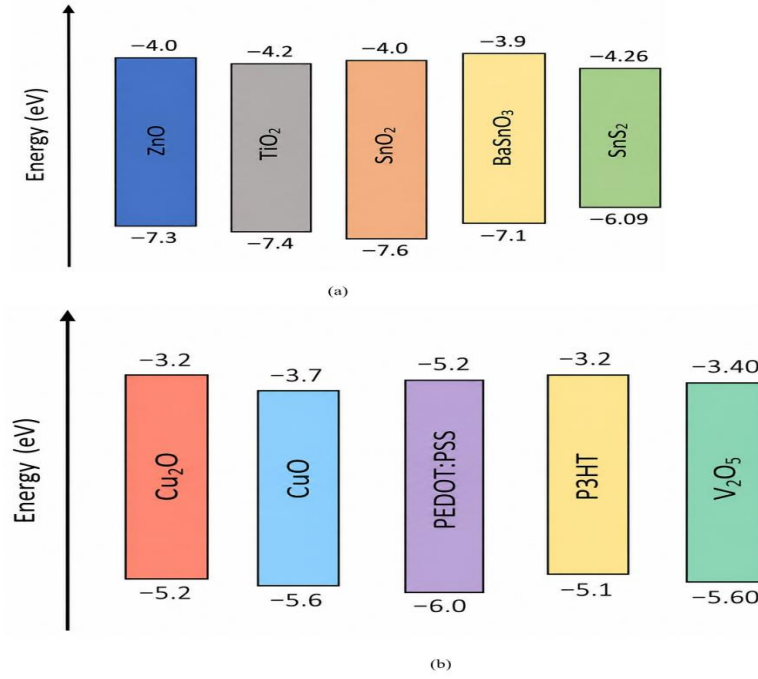


Fig. 2. Energy band diagrams of the various (a) ETLs, (b) HTLs.

2.2 PSC simulation parameters

The material parameters adopted for the device simulation are summarized in Tables 1 and 2 and were obtained from previously reported experimental and numerical studies [5, 29-37]. The corresponding defect parameters assigned to the ETL/absorber and absorber/HTL interfaces are presented in Table 3. A work function of 4.4 eV was specified for the fluorine-doped tin oxide (FTO) front contact [38]. All simulations were performed under an incident illumination intensity of 1000 W/m², an AC frequency of 1 Hz, an applied voltage sweep from 0 to 1.50 V, and an operating temperature of 300 K (25 °C) [29, 32].

Table 1. Simulation input parameters of FTO, absorber layer (Cs_{0.05}FA_{0.79}MA_{0.15}PbI_{2.45}Br_{0.55}, referred as CsFAMAPbIBr), and ETLs

Parameters	Layer						
	FTO [29]	Absorber [5]	BaSnO ₃ [30, 31]	IGZO [32]	SnS ₂ [33]	TiO ₂ [39]	PCBM [32]
Thickness (μm)	0.5	0.6	0.01	0.1	0.01	0.01	0.1

E_g (eV)	3.5	1.6	3.16	3.05	1.85	3.2	2.0
χ (eV)	4.3	3.9	3.90	4.16	4.26	4.2	3.9
ϵ_r	9.0	6.6	17.0	10.0	17.7	10.0	3.9
N_C (cm ⁻³)	2.2×10^{18}	1.0×10^{18}	1.2×10^{19}	5.0×10^{18}	7.32×10^{18}	2.2×10^{18}	2.5×10^{21}
N_V (cm ⁻³)	1.8×10^{19}	1.0×10^{18}	1.8×10^{19}	5.0×10^{18}	1.8×10^{19}	2.2×10^{18}	1.5×10^{21}
μ_n (cm ² V ⁻¹ s ⁻¹)	200	2.0	200	8.0×10^{-2}	20	20	0.2
μ_p (cm ² V ⁻¹ s ⁻¹)	10	2.0	25	15	10	10	0.2
$e V_{th}$ (cm/s)	1×10^7	1×10^7	1×10^7	0.1	1×10^7	1×10^7	1×10^7
$h V_{th}$ (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
N_D (cm ⁻³)	1×10^{19}	0	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{15}
N_A (cm ⁻³)	0	1×10^{16}	0	0	0	0	0
N_t (cm ⁻³)	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{15}
σ (e) (cm ²)	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}
σ (h) (cm ²)	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}

Table 2. Simulation input parameters for the various HTL

Parameter	Layer				
	Cu ₂ O [34]	P ₃ HT [32]	V ₂ O ₅ [35-37]	CuO [34]	PEDOT [33]
Thickness (μ m)	0.2	0.5	0.5	0.5	0.5
E_g (eV)	2.17	1.7	2.2	1.5	1.70
χ (eV)	3.20	3.5	3.4	4.07	3.50
ϵ_r	7.11	6.5	8.0	18.1	3.0
N_C (cm ⁻³)	2.0×10^{18}	2.0×10^{18}	3.9×10^{19}	2.0×10^{18}	2.0×10^{18}
N_V (cm ⁻³)	1×10^{19}	2.0×10^{19}	5.0×10^{20}	1.0×10^{19}	2.0×10^{19}
μ_n (cm ² V ⁻¹ s ⁻¹)	80	1.8×10^{-3}	1×10^7	100	1.8×10^{-3}
μ_p (cm ² V ⁻¹ s ⁻¹)	80	1.8×10^{-2}	1×10^7	0.1	1.8×10^{-2}
$e V_{th}$ (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
$h V_{th}$ (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
N_D (cm ⁻³)	0	0	0	0	0
N_A (cm ⁻³)	1×10^{15}	1×10^{16}	1×10^{16}	1×10^{16}	1×10^{16}
N_t (cm ⁻³)	1×10^{15}	1×10^{14}	1×10^{15}	1×10^{15}	1×10^{15}
σ (e) (cm ²)	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}
σ (h) (cm ²)	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}

Table 3. Input interface defect parameters [32, 39]

Parameters	ETL / Absorber	Absorber / HTL
Defect type	Neutral	Neutral
σ (e) (cm ²)	1×10^{-19}	1×10^{-19}
σ (h) (cm ²)	1×10^{-19}	1×10^{-19}
Energetic distribution	Single	Single
Energy level with respect to E_v (eV)	0.60	0.60
Characteristic energy (eV)	0.10	0.10
Interface defect density (cm ⁻²)	1×10^{12}	1×10^{12}

Bulk and interfacial defect states were incorporated into the SCAPS-1D model using the Shockley-Read-Hall recombination formalism. A single neutral trap state was assigned to both the bulk layers and the interfaces. For the interface defects, the trap level was located at $E_v = +0.60$ eV with a characteristic energy of 0.10 eV. Meanwhile the electron and hole capture cross-sections, σ_n and σ_p , were each fixed at 1×10^{-15} cm² (Table 3). These parameters were adopted from published SCAPS-based PSC studies and designate recombination-active trap states suitable for assessing the effects of interface quality and defect passivation. During the optimization procedure, only the defect density was varied comprehensively, whereas the trap energy level and carrier capture cross-sections were maintained constant. This approach allowed the influence of trap concentration on the photovoltaic response to be evaluated independently.

3.0 Results and Discussion

3.1 Photovoltaic output of the initial PSCs

This section evaluates the photovoltaic response of the CsFAMAPbIBr-based PSC using different electron and hole transport layers. The FTO/BaSnO₃/CsFAMAPbIBr/Cu₂O/C configuration was first considered as the reference device, and its simulated photovoltaic metrics are presented in Table 3. Subsequently, the ETL and HTL materials were varied individually while maintaining the remaining device parameters unchanged. This comparative approach was used to determine the transport-layer combination that provides the most favorable charge collection, suppressed recombination losses, and photovoltaic performance.

3.1.1 Energy band alignment engineering of the prototype PSC using various ETLs and HTLs

Energy-band alignment at the absorber/transport-layer interfaces plays a major role in determining carrier extraction and recombination in PSCs. Appropriate selection of ETL and HTL materials can therefore be used to engineer the interfacial energetics and improve device performance [5]. At the absorber/ETL interface, the conduction-band offset (CBO) is described by the difference between the conduction-band minima of the perovskite absorber and the ETL [40, 41]. This offset governs electron transport across the interface and influences electron accumulation and recombination. Similarly, the valence-band offset (VBO) is determined from the difference between the valence-band maxima of the absorber and HTL and controls the energetic barrier encountered during hole extraction [42]. Consequently, favorable CBO and VBO values are required to provide preferential carrier transport while suppressing recombination at the interface. The calculated band offsets for the investigated ETLs and HTLs are presented in Tables 4 and 5.

Table 4. Influence of ETL on performance metrics of the prototype PSC

Solar cell	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
FTO/BaSnO ₃ /CsFAMAPbIBr/Cu ₂ O/C	1.24	21.47	74.79	19.91
FTO/IGZO/CsFAMAPbIBr/Cu ₂ O/C	1.24	0.14	92.17	0.16
FTO/SnS ₂ /CsFAMAPbIBr/Cu ₂ O/C	1.21	21.46	74.15	19.19
FTO/PCBM/CsFAMAPbIBr/Cu ₂ O/C	1.24	21.39	74.49	19.73
FTO/TiO ₂ /CsFAMAPbIBr/Cu ₂ O/C	1.23	21.44	74.56	19.69

Table 5. Impact of HTL on photovoltaic metrics of the prototype PSC

Solar cell	V_{OC} (V)	J_{SC} (mA/cm ²)	FF (%)	PCE (%)
FTO/BaSnO ₃ /CsFAMAPbIBr/Cu ₂ O/C	1.24	21.47	74.79	19.91
FTO/BaSnO ₃ /CsFAMAPbIBr/CuO/C	1.03	20.64	73.43	15.60
FTO/BaSnO ₃ /CsFAMAPbIBr/PEDOT:PSS/C	0.58	18.75	32.08	3.47
FTO/BaSnO ₃ /CsFAMAPbIBr/P ₃ HT/C	1.08	21.05	71.54	16.32
FTO/BaSnO ₃ /CsFAMAPbIBr/V ₂ O ₅ /C	1.15	20.73	74.21	17.69

The influence of the transport layers was first examined by varying the ETL in the initial FTO/BaSnO₃/CsFAMAPbIBr/Cu₂O/C device, while keeping Cu₂O HTL unchanged. As shown in Table 4, the FTO/BaSnO₃/CsFAMAPbIBr/Cu₂O/C PSC produced a superior response, with a PCE of 19.91%. The PCBM- and TiO₂-based devices followed closely, with PCEs of 19.73% and 19.69%, respectively, whereas SnS₂ yielded a slightly lower PCE of 19.19% (Table 4). The small variation in J_{SC} (Fig. 3a) among BaSnO₃, SnS₂, PCBM, and TiO₂ indicates that these ETLs have little influence on the amount of photogenerated current (Table 4). Their main effect is associated with electron extraction, interfacial recombination, and the resulting changes in V_{OC} and FF.

The outstanding performance of BaSnO₃ agrees with its suitable conduction-band alignment with the CsFAMAPbIBr absorber. Both materials have conduction-band minima close to -3.90 eV, producing an approximately zero CBO. Such alignment mitigates the energy barrier for electron transfer from the absorber into the ETL and reduces carrier accumulation at the interface. PCBM possesses a similarly favorable conduction-band position and consequently gives a PCE close to that obtained with BaSnO₃. Nevertheless, the slightly higher performance of BaSnO₃ can also be associated with its stronger electron-transport characteristics under the input parameters adopted in the simulation (Table 1). TiO₂ and SnS₂, with conduction-band minima located deeper than that of the absorber, introduce larger conduction-band discontinuities. This is reflected particularly in the slightly lower V_{OC} values of 1.23 and 1.21 V, respectively, and the corresponding reduction in device efficiency.

A distinctly different response is observed for the IGZO-based device. Although a relatively high V_{OC} of 1.24 V and FF of 92.17% are obtained, the J_{SC} collapses to only 0.14 mA/cm²

(Fig. 3b), resulting in a very low PCE of 0.16%. Therefore, the unusually high FF does not translate into useful photovoltaic performance because the maximum obtainable power is severely limited by the extremely small photocurrent. This behaviour suggests that, under the adopted IGZO parameters, electron collection or transport is strongly restricted. The result also emphasizes that a high V_{OC} or FF alone is insufficient to guarantee an efficient solar cell; all three photovoltaic quantities, particularly J_{SC} , must be sufficiently high. Based on the photovoltaic response, $BaSnO_3$ is selected as the most suitable ETL for the subsequent HTL comparison.

With $BaSnO_3$ fixed as the ETL, Cu_2O , CuO , PEDOT:PSS, P3HT, and V_2O_5 are then investigated as alternative HTLs (Table 2). Table 5 shows a much stronger dependence of device performance on the HTL than was observed for most of the ETLs. Cu_2O again produces the best device, maintaining a PCE of 19.91%. V_2O_5 is the second-best HTL, delivering a PCE of 17.69%. P3HT produced an intermediate efficiency of 16.32%, while the CuO -based cell decreased further to 15.60%. The weak quantum efficiency (QE) spectrum of the IGZO-based cell (Fig. 3c) supports the very low J_{SC} , indicating that photon absorption, carrier generation and extraction is low. Whereas, the overlapping QE spectra of the other ETL supports the equivalent J_{SC} delivered these PSCs, suggesting identical photon harvesting and carrier generation.

The favorable performance of Cu_2O can be ascribed to the combined effects of suitable valence-band alignment, carrier selectivity, and hole transport. The valence-band maximum of the CsFAMAPbIBr absorber is approximately -5.50 eV, whereas Cu_2O has a valence-band level near -5.37 eV. The resulting small valence-band discontinuity provides a relatively favorable pathway for holes to leave the absorber while still maintaining carrier selectivity at the rear interface. This helps suppress excessive hole accumulation and recombination, thereby supporting the higher V_{OC} , FF, and PCE (Table 5). V_2O_5 also demonstrates a valence-band edge close to that of the absorber, which accounts for its reasonably good photovoltaic response. Nevertheless, its V_{OC} and J_{SC} are lower than those obtained with Cu_2O , reducing the PCE from 19.91% to 17.69%. P3HT similarly maintains a relatively high J_{SC} of 21.05 mA/cm² (Fig. 3d), but its lower V_{OC} and FF of 71.54% limit the PCE to 16.32%. These results indicate that sufficient photogeneration is retained in the P3HT device, while voltage and transport-related losses account for most of the efficiency reduction. The equivalent higher QE spectral of the Cu_2O - and P3HT-based cells (Fig. 3e) supports the equivalent and higher J_{SC} delivered by the solar cells, indicating that photon absorption, carrier

generation is the same. On the hand, the PEDOT:PSS-based cell exhibits the least QE, which explains the lower J_{SC} obtained from this device due to poor light harvesting and carrier generation.

For CuO HTL, the reduction of V_{OC} to 1.03 V and J_{SC} to 20.64 mA/cm² lowers the PCE to 15.60%, despite maintaining a relatively good FF of 73.43%. This demonstrates that favorable valence-band alignment alone does not determine HTL performance. Carrier mobility, doping, bulk and interface defects, and the energetic interaction between the HTL and carbon electrode can also influence hole extraction and recombination. The most severe deterioration occurred for PEDOT:PSS, where V_{OC} , J_{SC} , and FF dropped substantially, producing a PCE of only 3.47%. The simultaneous suppression of V_{OC} and FF indicates substantial recombination and/or poor carrier-selective transport within the device configuration. The reduction in J_{SC} further suggests less efficient hole collection, causing photogenerated carriers to be lost before reaching the external circuit.

The results indicates that the FTO/BaSnO₃/CsFAMAPbIBr/Cu₂O/C architecture is the hero prototype device for the subsequent optimization studies. This is because it provides the best balance of carrier extraction, interfacial selectivity, and recombination mitigation, yielding a PCE of 19.91%.

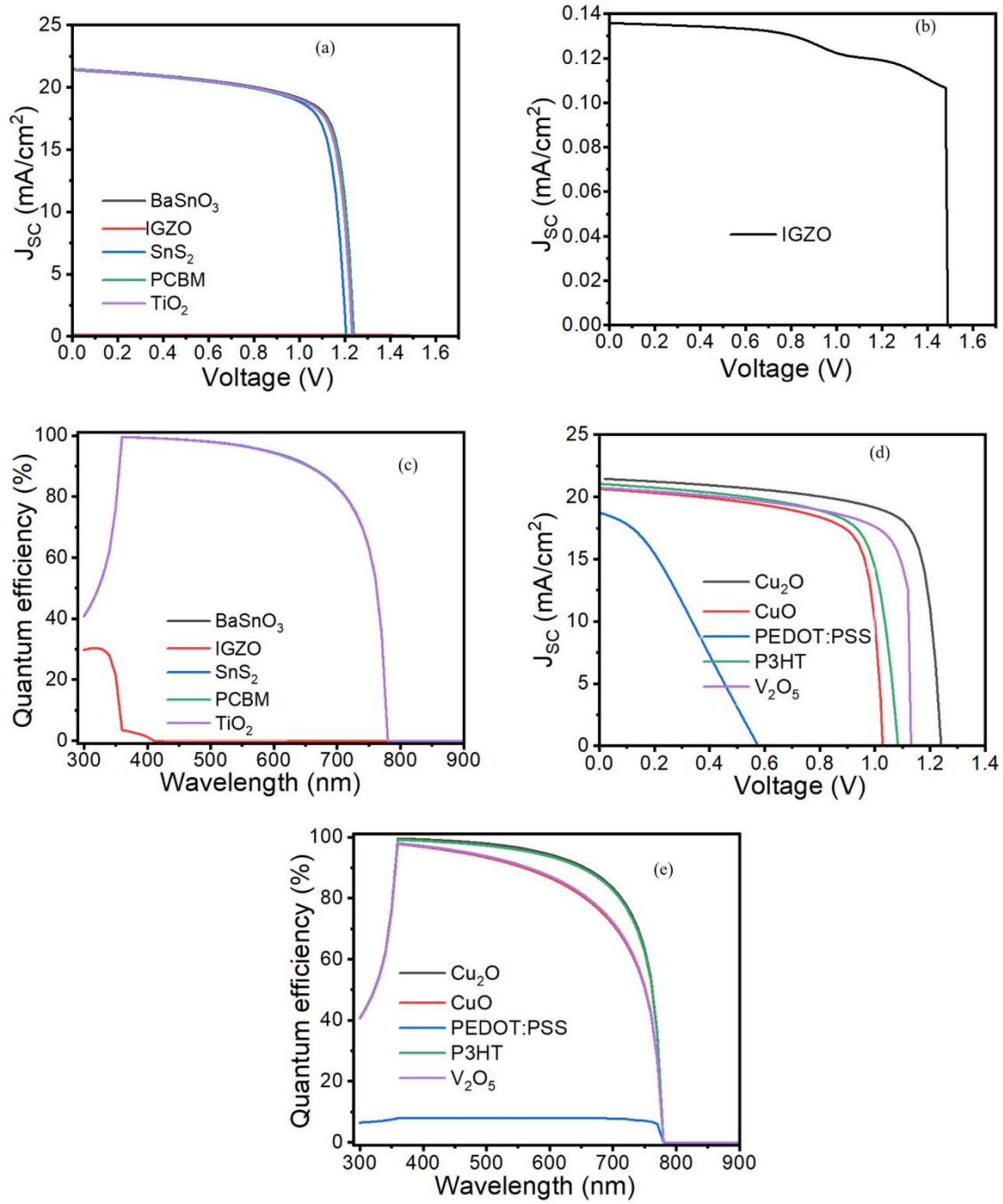


Fig. 3. J-V characteristics for various ETLs, (b) Zoom-in J-V characteristics for IGZO ETL, (c) QE spectra for various ETLs, (d) J-V characteristics for various HTLs, (e) QE spectra for various HTLs

3.1.2 Photovoltaic output of the best prototype solar cell

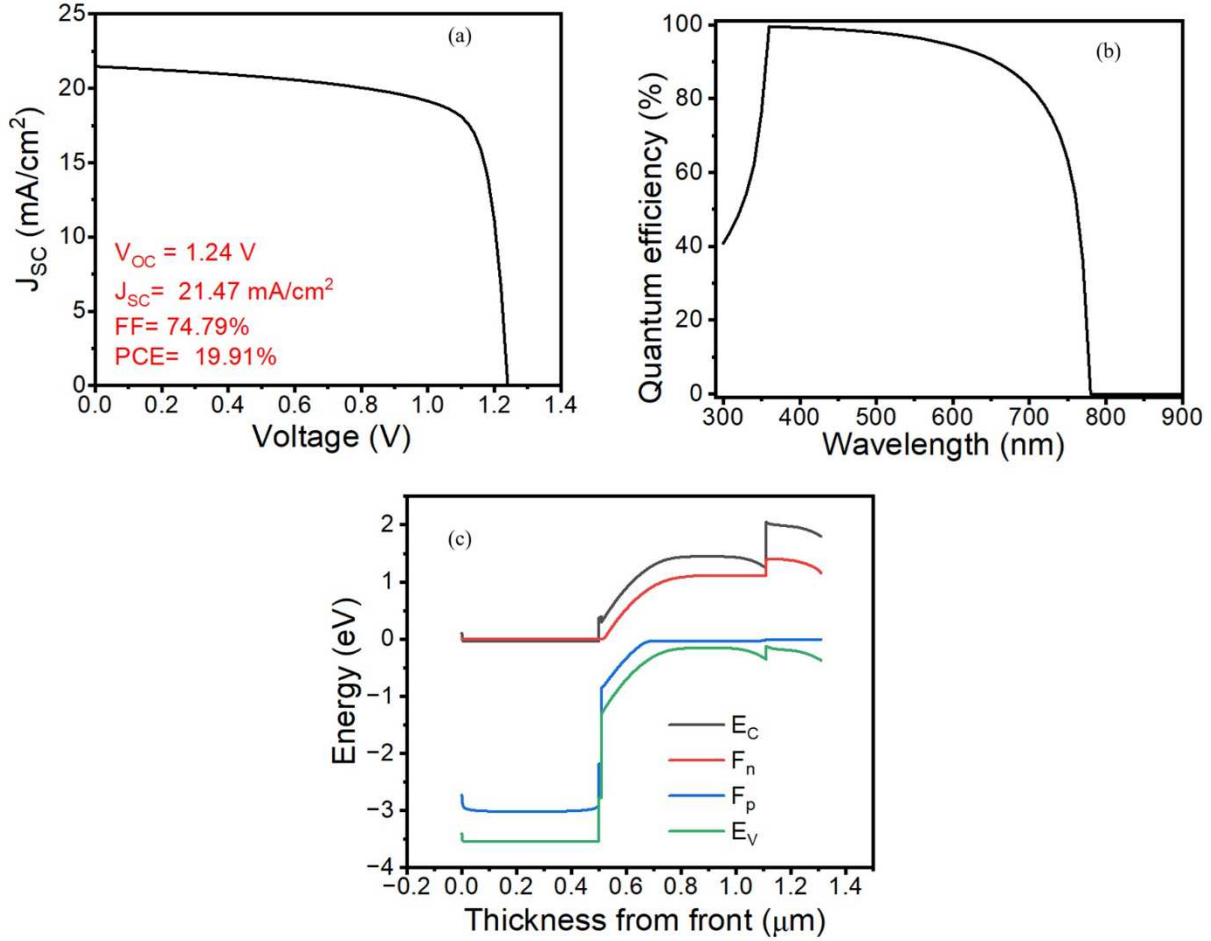


Fig. 4. (a) Energy band plot of the prototype CBTS HTL-assisted PSC, (b) QE plot, (c) Energy band of the CBTS HTL-assisted cell, (d) Carrier generation rate, (e) Recombination rate.

3.2 Effect of varying BaSnO_3 ETL thickness

The thickness of the BaSnO_3 ETL was varied from 0.02 to 0.06 μm while the other device parameters were maintained unchanged. Over this range, V_{oc} remains constant at 1.24 V, whereas J_{sc} decreases slightly from 21.44 to 21.31 mA/cm^2 , FF decreases from 74.69 to 74.35%, and the PCE consequently falls from 19.85 to 19.64% (Fig. 5a). The weak variation indicates that BaSnO_3 thickness is not a dominant performance-limiting parameter within the investigated range.

The constant V_{oc} can be attributed to the unchanged energetic alignment and defect properties at the $\text{BaSnO}_3/\text{CsFAMAPbIBr}$ interface as the ETL thickness varies. Since both

materials have conduction-band edges close to (-3.90) eV, the nearly zero CBO preserves efficient electron extraction, while the recombination balance and quasi-Fermi-level splitting remain essentially unchanged. The constant V_{OC} and nearly unchanged ratio of photogenerated current density (J_{ph}) to reverse saturation current density (J_0) with the varying $BaSnO_3$ thickness are related by Eq. 10 [13].

$$V_{OC} = \frac{nkT}{q} \ln \left(\frac{J_{ph}}{J_0} + 1 \right), \quad 10$$

where n the ideality factor, q is electron charge, k is Boltzmann constant, and T is temperature. The small reduction in J_{SC} can be ascribed to the longer electron-transport path created by increasing the $BaSnO_3$ thickness. A thicker ETL increases the distance electrons must travel before reaching the FTO contact, thereby increasing transport resistance and the probability of carrier loss. This behaviour is consistent with Eq. 11, which shows that the electrical resistance of a uniformly conducting ETL increases with its thickness [14, 43]. Nevertheless, the effect is little because $BaSnO_3$ possesses favourable electron-transport properties (Table 1). The overlapping quantum efficiency (QE) spectra (Fig. 6a) support the nearly steady J_{SC} , indicating that light harvesting, charge generation and collection has not change.

$$R_{ETL} = \frac{\rho t_{ETL}}{A} = \frac{t_{ETL}}{q\mu_n n A}, \quad 11$$

where R_{ETL} is electrical resistance of the $BaSnO_3$ ETL, ρ is electrical resistivity of the ETL, t_{ETL} , is thickness of the ETL, A represent cross-sectional area through which the electrons flow, q is elementary charge, μ_n is electron mobility in $BaSnO_3$, n is free-electron concentration, and σ is electrical conductivity ($\sigma = 1/\rho$)

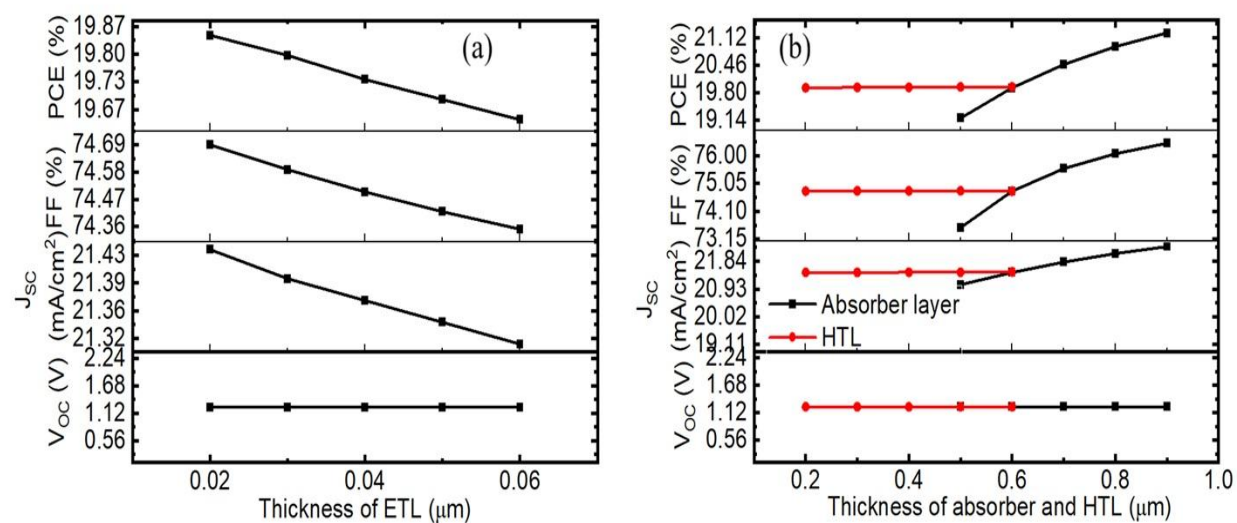


Fig. 5. Variation of V_{oc} , J_{sc} , FF, and PCE with thickness of the (a) ETL, (b) Absorber and HTL.

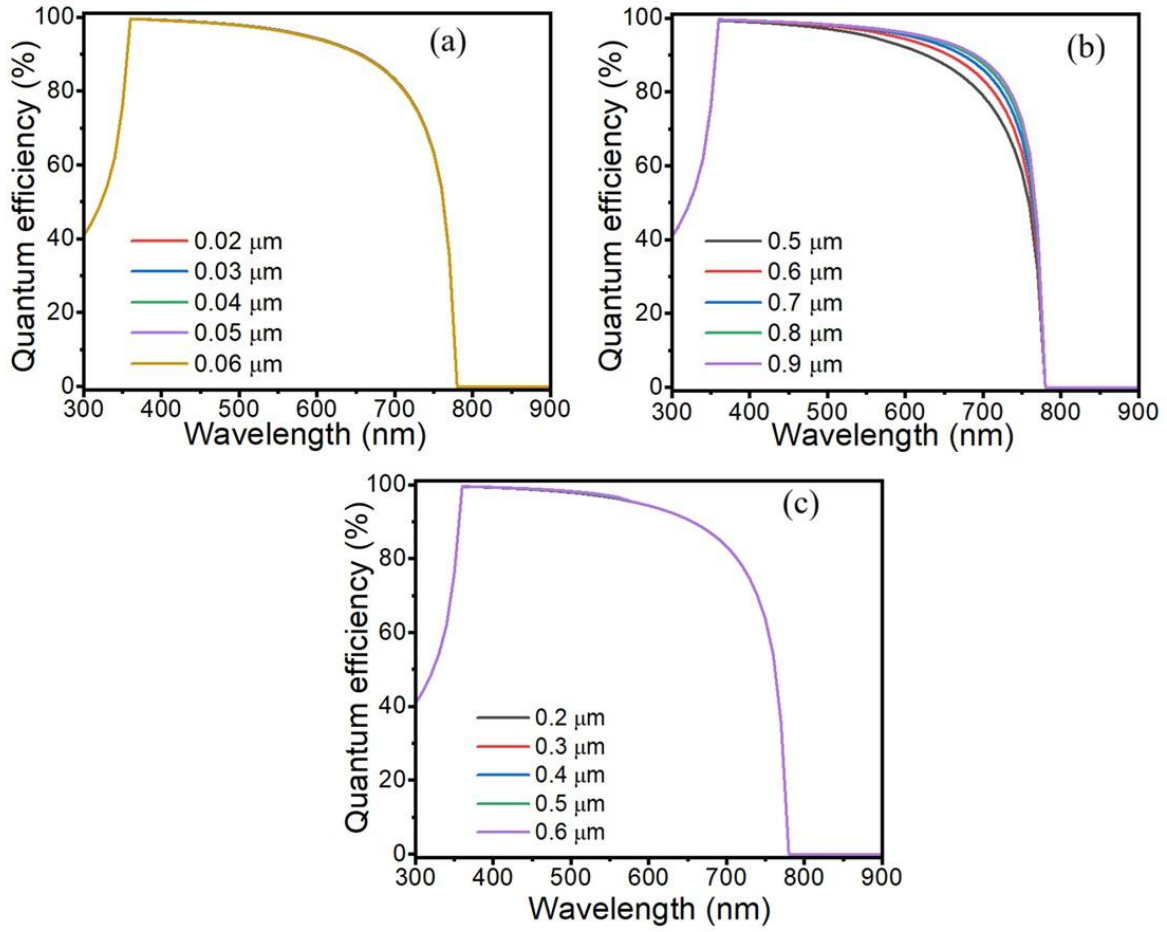


Fig. 6. Quantum efficiency spectra for the varying thickness of (a) ETL, (b) Absorber, (c) HTL

The slight decrease in FF (74.69 - 74.35%) can also be attributed to the increased transport resistance of the thicker ETL. The resulting additional voltage drops under current flow, particularly near the maximum-power point, slightly reduces the squareness of the J-V curve. The PCE is given by Eq. 12, therefore, the slight reduction in PCE can be traced to the decrease in J_{SC} and FF because V_{OC} remained constant.

$$PCE = \frac{V_{OC} \times J_{SC} \times FF}{P_{in}}, \quad 12$$

where V_{OC} and J_{SC} denote open circuit voltage, short circuit current density, and P_{in} is incident power density. Based on the results, the 0.02 μm thickness is selected for subsequent optimization because of its higher performance metrics.

3.3 Effect of varying absorber thickness

Fig 5b shows that increasing the CsFAMAPbIBr absorber thickness from 0.5 to 0.9 μm increases J_{SC} from 21.07 to 22.32 mA/cm^{-2} , FF from 73.54 to 76.43%, and PCE from 19.18 to 21.23%, while V_{OC} remains constant at 1.24 V. The improvement can be traced to improved photon absorption and carrier collection in the thicker absorber.

The increase in J_{SC} can be attributed to the longer optical path provided by the thicker CsFAMAPbIBr layer. According to the Beer-Lambert relation (Eq. 13) [44]. Increasing the absorber thickness allows a greater proportion of incoming photons to be absorbed and converted into electron-hole pairs, thereby increasing J_{SC} . The smaller incremental gain at larger thicknesses indicates the progressive saturation of absorption within strongly absorbing spectral regions. The increase in QE spectra (Fig. 6b) in around 600 – 750 nm support the increase in J_{SC} due to increase in photon harvesting, carrier generation and extraction.

$$I(x) = I_0 e^{-\alpha x}, \quad 13$$

where I_0 designate the incident light intensity, α denote the absorption coefficient, and x is the penetration depth.

The constant V_{OC} can be attributed to the unchanged recombination balance and quasi-Fermi-level splitting over the investigated thickness range. Although the thicker absorber produces more photocarriers, the additional carrier population does not introduce sufficient recombination to cause a measurable voltage loss [45]. The increase in FF (73.54 - 76.43%) indicates that carrier extraction remains effective as the absorber thickness increases. This indicate that the carrier lifetime and transport properties are sufficient for photogenerated carriers to reach the selective contacts before undergoing recombination. The increase in PCE (19.18 to 21.23%) results mainly from the higher J_{SC} and FF. Thus, 0.9 μm is the best absorber thickness within the investigated range, although it should not be regarded as an absolute optimum because the PCE is still increasing at the upper limit of the thickness sweep.

3.4 Impact of changing Cu₂O HTL thickness

Fig. 5b shows that varying the Cu₂O thickness from 0.2 to 0.6 μm has a negligible effect on the photovoltaic response. V_{OC} remains at 1.24 V, J_{SC} changes only from 21.47 to 21.49 mA/cm^2 , FF stays $\sim 74.8\%$, and PCE increases slightly from 19.91 to 19.93%. This indicates that 0.2 μm Cu₂O is already sufficient to support effective hole extraction and carrier selectivity. The constant V_{OC} can be ascribed to the unchanged CsFAMAPbIBr/Cu₂O interfacial energetics and recombination conditions as the HTL thickness varies. The valence-band alignment remains fixed, therefore, changing only the physical thickness of Cu₂O does not appreciably alter hole-transfer energetics or the separation between the electron and hole quasi-Fermi levels within the absorber.

The nearly unchanged J_{SC} indicates that hole collection is not limited by Cu₂O thickness within the investigated thickness range, as supported by then overlapping QE spectra (Fig. 6c). The illumination enters through the FTO/BaSnO₃ side and photogeneration occurs mainly in the CsFAMAPbIBr absorber therefore, increasing the rear Cu₂O thickness has little influence on photon absorption or carrier generation. The constant FF shows that thicker Cu₂O does not introduce a significant additional transport penalty. This behaviour is consistent with the relatively high carrier mobility assigned to Cu₂O, which allows holes to reach the carbon contact without substantial resistive loss. Consequently, the PCE changes by only 0.02 percentage points. Thus, Cu₂O thickness is a highly tolerant fabrication parameter within the investigated 0.2–0.6 μm range.

3.5 Effect of carrier concentration

3.5.1 Impact of carrier concentration of the ETL

Increasing the BaSnO₃ donor concentration from 10^{14} to 10^{17} cm^{-3} produces only a slight improvement in device performance. V_{OC} remains constant at 1.24 V, J_{SC} changes marginally from 21.47 to 21.48 mA/cm^2 , FF increases from 74.79 to 75.01%, and PCE rises from 19.90 to 19.97% (Fig. 7). For an n-type ETL with fully ionized donors ($n \approx N_{\text{D}}$), the electrical conductivity is given by Eq. 14 [46, 47].

$$\sigma_n = qn\mu_n \approx qN_{\text{D}}\mu_n, \quad 14$$

where q is the elementary charge, n is the electron density and μ_n is the electron mobility. Thus, increasing donor concentration (N_{D}) raises the conductivity and lowers the resistivity of BaSnO₃. For

an ETL of fixed thickness, the area-normalized transport resistance can be expressed approximately as Eq. 11 [48]. This shows that a higher electron concentration reduces the resistance to electron transfer. This boosts electron extraction from the CsFAMAPbIBr absorber toward the FTO contact and accounts for the small increase in FF. An increase in the donor concentration also shifts the electron Fermi level toward the conduction-band edge according to Eq. 15 [46].

$$E_C - E_F = k_B T \ln \left(\frac{N_C}{n} \right), \quad 15$$

where E_C is the conduction-band edge, E_F is the Fermi level, and N_C is the effective conduction-band density of states. The resulting higher n-type character can improve electron selectivity. However, BaSnO₃ already forms a favourable, nearly zero CBO with CsFAMAPbIBr, therefore further doping provides a limited additional improvement to interfacial electron transfer.

The constant V_{OC} indicates that the donor-density variation has little effect on the dominant recombination processes and the separation between the electron and hole quasi-Fermi levels. The unchanged J_{SC} confirms that photon absorption and carrier generation in the absorber are essentially unaffected by BaSnO₃ doping. The principal effect is the reduction of electron-transport resistance, reflected mainly in the slight improvement in FF. The results indicates that 10^{17} cm^{-3} is the best doping value because it gives the highest PCE of 19.97% within the investigated range.

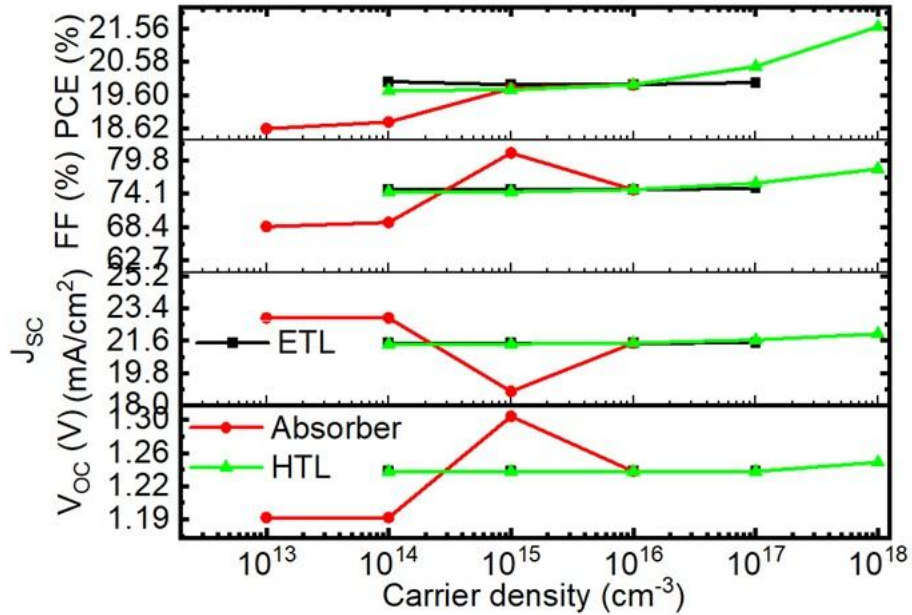


Fig. 7. Variation of V_{OC} , J_{SC} , FF, and PCE with carrier density of the various layers.

3.5.2 Influence of carrier density of the absorber layer

The absorber carrier concentration produces a non-monotonic photovoltaic response. Increasing carrier concentration from 10^{13} to 10^{16} cm^{-3} raises the PCE from 18.61 to 19.91%, although V_{OC} , J_{SC} , and FF vary differently (Fig. 7). At 10^{15} cm^{-3} , V_{OC} and FF reach 1.30 V and 81.08%, respectively, while J_{SC} falls to 18.77 mA/cm^2 . At 10^{16} cm^{-3} , J_{SC} recovers to 21.47 mA/cm^2 , giving the highest PCE of 19.91%. An increase in the acceptor carrier density increases the hole conductivity according to Eq. 16.

$$\sigma_p = qn\mu_p \approx qN_A\mu_p, \quad 16$$

where N_A denote the acceptor concentration, and N_A is acceptor carrier density. A higher carrier concentration lowers the absorber resistivity and improve hole transport, which contribute to the improvement in FF.

The carrier concentration also modifies the depletion-region width and the associated electric field. The depletion width for a one-sided abrupt-junction approximation can be expressed using Eq. 17. [49]. This shows that an increase in the effective doping concentration reduces the depletion width. The associated redistribution of the electric field changes the balance between field-assisted carrier separation and transport through the quasi-neutral region [50].

$$W = \sqrt{\frac{2\varepsilon(V_{bi} - V)}{qN_{eff}}} \quad 17$$

where W is depletion-region width, ε is absolute permittivity of the semiconductor, V_{bi} is built-in potential of the junction, V is externally applied voltage, q designates elementary charge, and N_{eff} is effective doping or ionized carrier concentration controlling the depletion region.

The reduction of J_{SC} to 18.77 mA/cm^2 at 10^{15} cm^{-3} , followed by its recovery at 10^{16} cm^{-3} , can be linked to competing impacts of conductivity, depletion width, electric-field distribution, carrier collection, and recombination [51]. The response should not be interpreted as a simple increase in performance with doping.

The high V_{OC} and FF at 10^{15} cm^{-3} indicate favourable voltage preservation and charge extraction, but the accompanying photocurrent loss limits the PCE to 19.80%. At 10^{16} cm^{-3} , the recovery of J_{SC} provides a better balance, yielding V_{OC} , J_{SC} , FF, and PCE of 1.24 V, 21.47 mA/cm^2 , 74.79%, and the highest 19.91%, respectively. Thus, 10^{16} cm^{-3} is chosen as the best absorber carrier concentration within the investigated range.

3.5.3 Effect of carrier concentration of the Cu_2O HTL

Fig. 7 shows that increasing the Cu_2O acceptor carrier density from 10^{14} to 10^{18} cm^{-3} steadily improves the device performance. V_{OC} increases from 1.24 to 1.25 V, J_{SC} from 21.41 to 21.99 mA/cm^2 , and FF from 74.39 to 78.34%, which raise the PCE from 19.74 to 21.62%. The improvement is controlled mainly by the increase in FF, with smaller contributions from J_{SC} and V_{OC} . The improvement can be ascribed to the higher hole conductivity of p-type Cu_2O , according to Eq. 16.

An increase in acceptor carrier density lowers the resistivity of Cu_2O and provides a more conductive pathway for holes moving from the CsFAMAPbIBr absorber toward the carbon electrode. The increase in FF from 74.39 to 78.34% can be traced to the reduction in hole-transport losses. Higher Cu_2O conductivity reduces the voltage drop across the HTL and limits carrier accumulation near the $\text{CsFAMAPbIBr/Cu}_2\text{O}$ interface, producing a more rectangular J-V response.

The moderate rise in J_{SC} from 21.41 to 21.99 mA/cm^2 indicates improved carrier collection. Since photon absorption occurs predominantly in the CsFAMAPbIBr absorber, Cu_2O doping mainly affects the extraction of photogenerated holes. Faster hole transport reduces their residence time near the rear interface and lowers the probability of interfacial charge recombination. The small increase in V_{OC} to 1.25 V at 10^{18} cm^{-3} suggests a modest reduction in recombination losses at the absorber/ Cu_2O interface. The results shows that 10^{18} cm^{-3} is the optimal doping since it gives the best performance.

3.6 Effect of bulk defect density

3.6.1 Influence of defect density of ETL

Fig. 8 demonstrates that increasing the BaSnO_3 bulk defect density from 10^{14} to 10^{16} cm^{-3} produces negligible modification in the photovoltaic metrics. The V_{OC} , J_{SC} , FF and PCE remain constant at 1.24 V, 21.47 mA/cm^2 , 74.79% and 19.91%, respectively. Performance begins to deteriorate at

10^{17} cm^{-3} , where J_{SC} decreases slightly to 21.45 mA/cm^2 and PCE to 19.85%. At 10^{18} cm^{-3} , V_{OC} falls to 1.23 V, J_{SC} to 21.40 mA/cm^2 , and PCE to 19.64%, while FF remains essentially unchanged at about 74.7%.

The weak dependence at defect density of $\leq 10^{16} \text{ cm}^{-3}$ indicates that recombination within BaSnO_3 is not a major loss mechanism because it functions primarily as an electron-selective transport layer. In addition, its favourable conduction-band alignment with CsFAMAPbIBr and high electron mobility promote rapid electron extraction toward FTO, limiting the residence time of electrons within the ETL.

At defect density of $\geq 10^{17} \text{ cm}^{-3}$, the larger trap population increases the probability of Shockley-Read-Hall recombination. The carrier lifetime is approximately related to defect density by Eq. 9. An increase in defect density shortens the electron lifetime and slightly increases trapping and recombination during electron transport.

The main deterioration at high defect density is the small loss in J_{SC} , together with a slight reduction in V_{OC} at 10^{18} cm^{-3} . The FF changes by less than 0.1 percentage point, showing that the charge-transport characteristics of BaSnO_3 is largely preserved. As a result, the PCE decreases by only 1.36% across four orders of magnitude in defect density.

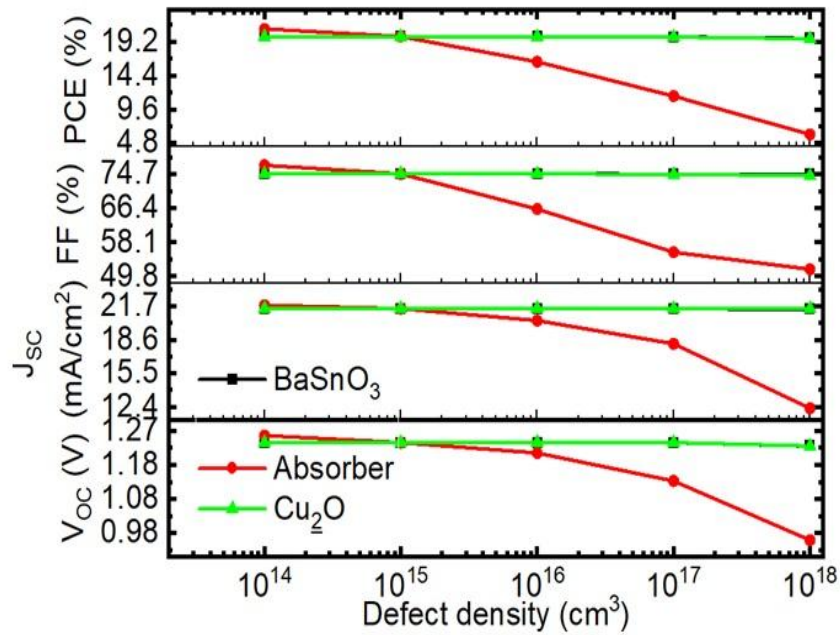


Fig. 8. Variation of V_{OC} , J_{SC} , FF, and PCE with bulk defect density of the various layers.

3.6.2 Impact of defect density of absorber layer

Fig. 8 shows that increasing the CsFAMAPbIBr bulk defect density from 10^{14} to 10^{18} cm^{-3} strongly deteriorates device performance. V_{OC} decreases from 1.26 to 0.96 V, J_{SC} from 21.77 to 12.27 mA/cm^2 , FF from 76.88 to 51.52%, and PCE from 21.01 to 6.04%. The sharp decline above 10^{15} cm^{-3} shows that bulk defects in the absorber are a major source of recombination loss. The deterioration can be ascribed to the increase in number of trap states within the absorber bandgap, which enhance Shockley-Read-Hall recombination [52]. The carrier lifetime varies approximately as Eq. 9 since the trap energy and capture cross-sections are fixed in the model, Thus, increasing defect density shortens the carrier lifetime and increases the likelihood of non-radiative recombination to occur before charge extraction [53].

The reduced lifetime also shortens the carrier diffusion length, according to Eq. 18 [44, 54]].

$$L_{n,p} = \sqrt{D_{n,p}\tau_{n,p}}, \quad 18$$

where $D_{n,p}$ is the electron or hole diffusion coefficient. Consequently, carriers generated within the absorber have a lower probability of reaching the selective contacts, which accounts for the strong decrease in J_{SC} , particularly at defect concentration of $\geq 10^{16} \text{ cm}^{-3}$.

The reduction in V_{OC} from 1.26 to 0.96 V can be attributed to the higher non-radiative recombination rate, which increases the dark saturation current and reduces the electron-hole quasi-Fermi-level splitting. The accompanying decrease in FF suggests stronger recombination under forward bias, which lowers the photocurrent around the maximum-power region and reduces the squareness of the J-V curve.

3.6.3 Effect of defect density of Cu_2O HTL

An increase in the Cu_2O bulk defect density from 10^{14} to 10^{16} cm^{-3} has small effect on device performance, with V_{OC} , J_{SC} , FF, and PCE of 1.24 V, 21.47 mA/cm^2 , 74.79%, and 19.91%, respectively. A substantial decline appears at higher defect densities. At 10^{18} cm^{-3} , V_{OC} decreases to 1.23 V, FF to 74.35%, and PCE to 19.58%, while J_{SC} remains nearly unchanged at 21.48 mA/cm^2 . The deterioration at high defect density can be traced to trap-assisted Shockley-Read-

Hall recombination within the Cu₂O HTL. According to Eq. 9, increasing defect density shortens the carrier lifetime and increases the probability of hole trapping and recombination during transport toward the carbon electrode.

The nearly unchanged J_{SC} shows that Cu₂O bulk defects have little influence on photogeneration, which occurs predominantly in the CsFAMAPbIBr absorber. Their effect is observed mainly through transport and recombination losses in the HTL. At high defect density, hole trapping can slow extraction and promote charge accumulation [55], producing the slight reductions in V_{OC} , FF, and PCE. The influence of Cu₂O defects is weaker because Cu₂O functions primarily as a HTL, therefore increasing defect density by four orders of magnitude reduces the PCE by only 0.33 percentage points (19.91 - 19.58%).

3.7 Influence of varied defect density at the various interface

3.7.1 Influence of defect density at ETL/absorber interface

Fig. 9 shows that increasing the BaSnO₃/CsFAMAPbIBr interface defect density from 10^{10} to 10^{14} cm⁻² produces a modest deterioration in device performance. V_{OC} remains constant at 1.24 V and J_{SC} at 21.47 mA/cm², while FF decreases from 74.81 to 72.80% and PCE falls from 19.92 to 19.35%. Increasing the interface defect concentration introduces additional trap states at the BaSnO₃/CsFAMAPbIBr heterointerface. These traps can capture electrons and holes and promote trap-assisted interfacial recombination. At higher defect densities, carrier accumulation near the interface may also increase, particularly under forward bias, thereby enhancing recombination losses around the maximum-power region [56]. This reduces the squareness of the J-V curve and accounts for the observed decline in FF.

The unchanged J_{SC} indicates that carrier extraction under short-circuit conditions remains efficient throughout the investigated defect-density range. Similarly, the constant V_{OC} suggests that the additional interfacial recombination is insufficient to cause a measurable reduction in quasi-

Fermi-level splitting. The weak response can also be linked to the favourable conduction-band alignment between BaSnO₃ and CsFAMAPbIBr. The conduction-band edges close to -3.90 eV and the nearly zero CBO provides little energetic barrier to electron transfer into the ETL.

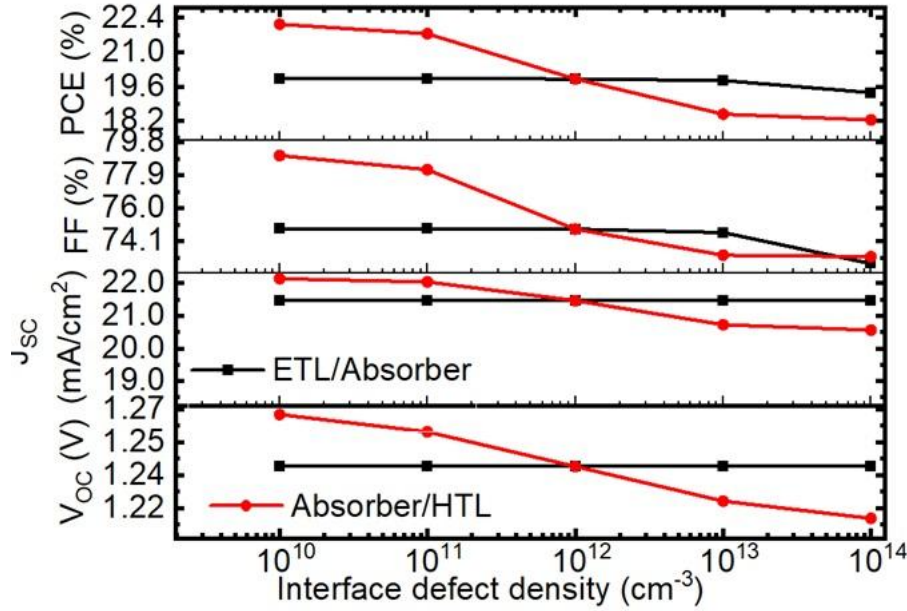


Fig. 9. Variation of V_{OC} , J_{SC} , FF, and PCE with defect density at the BaSnO₃/absorber and absorber/Cu₂O interfaces.

3.7.2 Influence of defect density at absorber/Cu₂O HTL interface

Fig. 9 shows that raising the CsFAMAPbIBr/Cu₂O interface defect density from 10^{10} to 10^{14} cm⁻² causes a marked deterioration in device performance. V_{OC} decreases from 1.27 to 1.21 V, J_{SC} from 22.14 to 20.56 mA/cm², FF from 79.04 to 73.20%, and PCE from 22.14 to 18.24%. The simultaneous decline in all photovoltaic parameters suggests that the absorber/Cu₂O interface is a significant recombination-sensitive region.

Higher interface defect density creates more trap states at the CsFAMAPbIBr/Cu₂O interface. These states enhance trap-assisted non-radiative recombination before holes are efficiently transferred into Cu₂O. The resulting carrier loss lowers J_{SC} , while the increased recombination rate reduces the electron-hole quasi-Fermi-level splitting and consequently decreases V_{OC} . The decrease in FF from 79.04 to 73.20% can likewise be attributed to stronger interfacial recombination and less efficient charge extraction under operating bias. Although the

CsFAMAPbIBr/Cu₂O interface provides favourable energetic conditions for hole transfer, a high density of interface traps can partly offset this advantage by increasing carrier trapping and recombination near the rear heterojunction [57]. Therefore, controlling the rear-interface defect density is considerably more crucial for device performance, and maintaining its magnitude at 10^{10} cm⁻² is beneficial for preserving efficient hole extraction, suppressing interfacial recombination, and sustaining high photovoltaic metrics.

3.8 Influence of absorber bandgap

Investigating the absorber bandgap is important because it determines the portion of the solar spectrum that can be harvested and sets the fundamental trade-off between J_{SC} and V_{OC} . Therefore, bandgap optimization is essential for maximizing the PCE of PSC [58-60]. The variation in bandgap among the CsFAMAPbIBr compositions arises from simultaneous changes in the halide and A-site cation ratios. Increasing the Br fraction relative to I generally widens the bandgap, while variations in the Cs/FA/MA ratio modify the perovskite lattice, Pb-halide bond geometry and octahedral tilting, which further shift the band-edge energies [59, 60, 62]. Bandgap of the absorber was varied from 1.60 –1.68 eV to investigate its impact of photovoltaic performance of the PSC.

Table 6. Influence of optical bandgap on performance metrics

Composition	Bandgap (eV)	V_{OC} (V)	J_{SC} (mA/cm ²)	FF (%)	PCE (%)
Cs _{0.05} FA _{0.79} MA _{0.15} PbI _{2.45} Br _{0.55}	1.60	1.24	21.47	74.79	19.91
Cs _{0.05} (FA _{0.83} MA _{0.17}) _{0.95} Pb(I _{0.83} Br _{0.17}) ₃	1.63	1.25	20.49	73.77	18.94
Cs _{0.05} MA _{0.15} FA _{0.80} Pb(I _{0.75} Br _{0.25}) ₃	1.65	1.26	19.78	73.33	18.27
Cs _{0.05} FA _{0.73} MA _{0.22} Pb(I _{0.77} Br _{0.23}) ₃	1.68	1.26	18.88	72.94	17.40

Table 6 and Fig. 10 shows that widening the CsFAMAPbIBr bandgap from 1.60 to 1.68 eV produces a slight increase in V_{OC} but a substantial reduction in J_{SC} . V_{OC} increases from 1.24 to 1.26 V, whereas J_{SC} decreases from 21.47 to 18.88 mA/cm². FF also declines from 74.79 to 72.94%, resulting in a reduction in PCE from 19.91 to 17.40%. The small increase in V_{OC} can be ascribed

to the larger energy separation available between the electron and hole quasi-Fermi levels in the wider-bandgap absorber [63, 64]. Increasing E_g also lowers the intrinsic carrier concentration and can reduce the dark saturation current, thereby supporting a higher photovoltage [65]. However, the increase in V_{OC} is little because the attainable voltage is also controlled by bulk and interfacial recombination losses.

The dominant effect of increasing bandgap is the reduction in J_{SC} . This reduction is supported by the decrease in the QE between 600 and 780 nm, indicating a decrease in the absorption edge (Fig. 10c). The bandgap and absorption-edge wavelength are related by Eq. 19.

$$E_g = \frac{hc}{\lambda_g} \quad 19$$

where E_g is bandgap, λ_g is absorption-edge or bandgap wavelength, h is Planck's constant, and c is speed of light in vacuum. Accordingly, increasing the bandgap from 1.60 to 1.68 eV shifts the absorption edge from approximately 775 to 738 nm. Photons with wavelengths beyond the corresponding absorption edge do not have sufficient energy to generate electron-hole pairs. This reduces the fraction of the solar spectrum available for photogeneration and consequently lowering J_{SC} .

The moderate decrease in FF (74.79 - 72.94%) indicates that the small voltage gain does not compensate for the photocurrent loss and the remaining recombination and transport losses under operating conditions. Therefore, PCE decreases monotonically as the bandgap increases. The bandgap of 1.60 eV provides the best balance between spectral absorption and photovoltage, yielding the highest PCE of 19.91%.

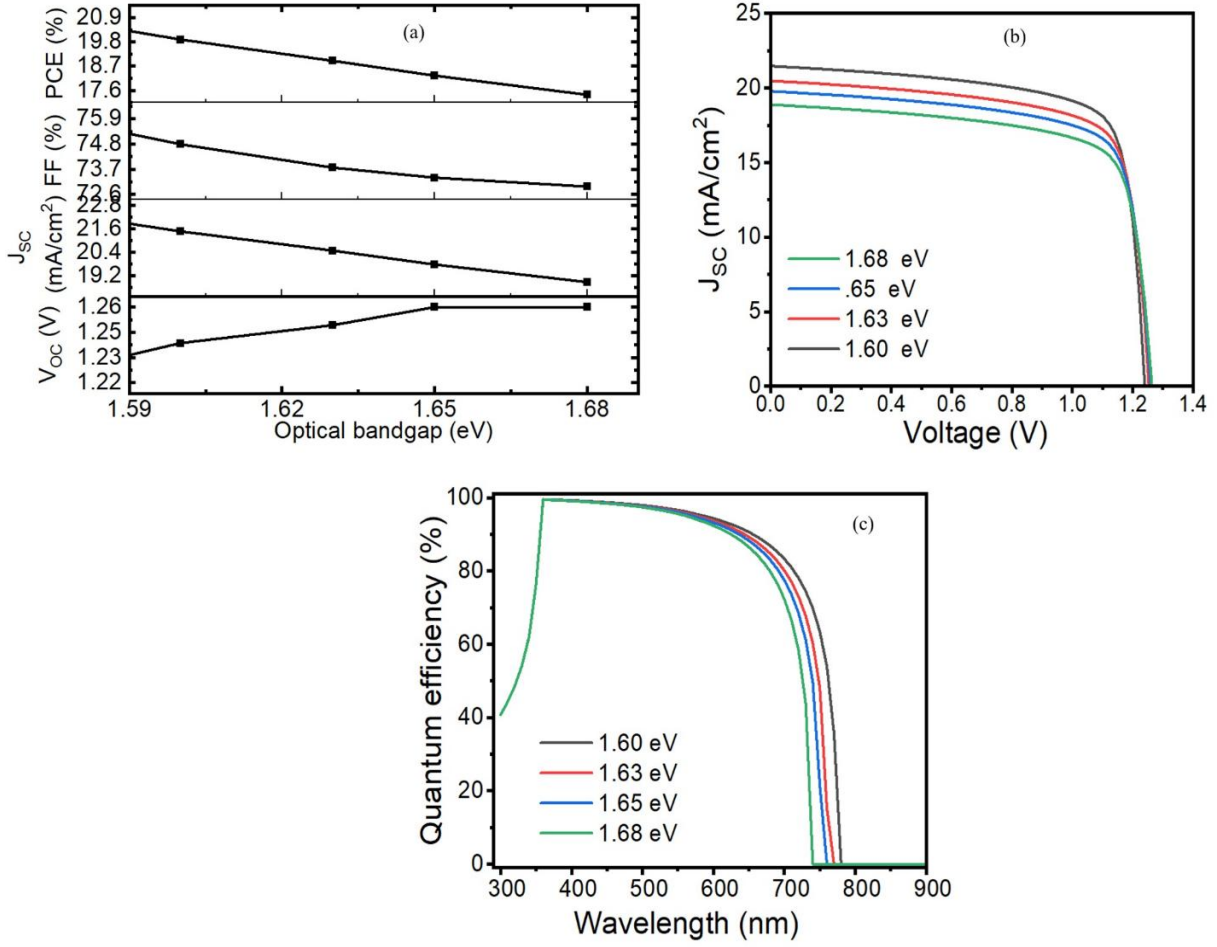


Fig. 10. Dependence of V_{OC} , J_{SC} , FF, and PCE on bandgap of the absorber, (b) J-V characteristics, (c) QE spectra.

3.9 Effect of resistance

3.9.1 Effect of series resistance

Series resistance in PSCs originates from the finite conductivity of the transparent conducting oxide (TCO) front electrode, ETL, absorber, HTL and rear electrode, together with contact/interfacial resistance at the TCO/ETL, ETL/perovskite, perovskite/HTL and HTL/rear-electrode interface. Poor interfacial contact, low carrier mobility and insufficient transport-layer conductivity can further increase series resistance, leading to FF and PCE losses [66, 67].

Increasing the series resistance from 1 to 4 Ωcm^2 causes a progressive decline in device performance. V_{OC} remains constant at 1.24 V, while J_{SC} declines slightly from 21.44 to 21.37

mA/cm² [Fig. 11a]. The strongest change occurs in the FF, which falls from 73.64 to 70.18%, reducing the PCE from 19.58 to 18.60%.

Series resistance produces an internal voltage loss under current flow, according to Eq. 20.

$$\Delta V = JR_s, \quad 20$$

where J is the current density and R_s is the area-normalized series resistance. An increase in series resistance dissipates a larger fraction of the photogenerated electrical energy inside the device without delivering to the external load.

The negligible change in V_{OC} is expected because the current is zero at open circuit; therefore, the voltage drop (Eq. 20) vanishes. In contrast, the effect of series resistance is important near the maximum-power region, where both current and voltage are appreciable. This explains why FF is most substantially affected.

The slight decrease in J_{SC} indicates that the investigated series resistance values are not large enough to severely restrict carrier collection under short-circuit conditions. Nevertheless, increasing resistance introduces a small additional transport loss, which account for the reduction from 21.44 to 21.37 mA/cm².

The associated resistive power loss can be expressed by Eq. 21. Thus, even a moderate increase in series resistance can noticeably reduce the power output when the device operates at high current density. The decline in PCE is therefore controlled mainly by the loss in FF. The results favour a low series resistance of about 1 Ωcm^2 to minimize internal voltage and power losses.

$$P_{loss} = J^2 R_s \quad 21$$

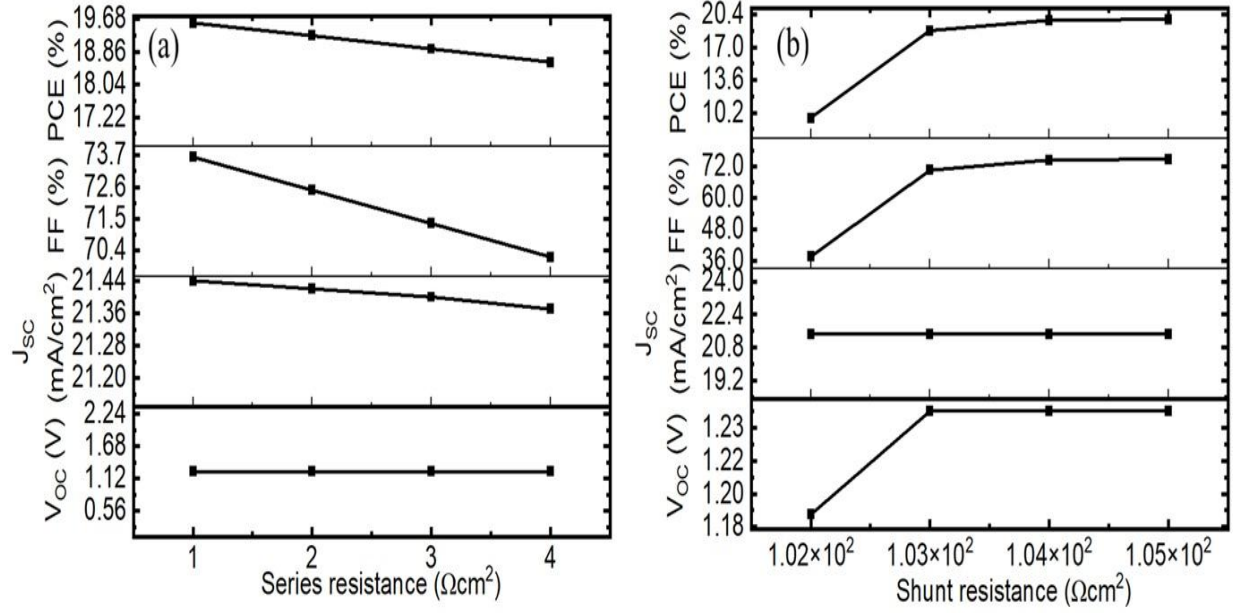


Fig. 11. Variation of V_{OC}, J_{SC}, FF, and PCE with (a) Series resistance, (b) Shunt resistance.

3.9.2 Impact of shunt resistance

Fig. 11b reveals that elevating the shunt resistance from 10^2 to $10^5 \Omega\text{cm}^2$ strongly improves device performance. V_{OC} increases from 1.19 to 1.24 V and FF from 37.66 to 74.75%, while J_{SC} remains essentially constant at 21.47 mA/cm². As a result, the PCE rises sharply from 9.66 to 19.90% (Fig. 11b), indicating that shunt leakage is a major loss mechanism at low shunt resistance.

Shunt resistance is associated with parasitic leakage pathways across the device. The corresponding leakage current density can be described by Eq. 22 [32], where V is the terminal voltage.

$$J_{sh} = \frac{V}{R_{sh}} \quad 22$$

A low shunt denote allows a significant fraction of the photogenerated current to bypass the external circuit. This leakage becomes particularly important under operating bias and severely reduces the squareness of the J-V curve, which explains the large deterioration in FF. The constant J_{SC} is expected because, under short-circuit conditions, $V = 0$, making J_{sh} very small [68]. In contrast, near the maximum-power region, the device operates at appreciable voltage, so leakage

through a low shunt resistance becomes substantial. This explains why FF is the most substantially affected.

The increase in V_{OC} from 1.19 to 1.24 V can also be traced to mitigation of leakage current. At low shunt resistance, part of the photogenerated current is internally lost through the shunt pathway, reducing the voltage that can be sustained under open-circuit conditions [69, 70]. Increasing shunt resistance suppresses this loss and allows a higher V_{OC} . Most of the improvement occurs between 10^2 and $10^4 \Omega\text{cm}^2$. Above $10^4 \Omega\text{cm}^2$, the photovoltaic parameters change only slightly, indicating that shunt leakage is no longer a dominant loss mechanism. The results suggest that, maintaining a high shunt resistance is critical for minimizing leakage losses and preserving high FF and PCE, with $10^5 \Omega\text{cm}^2$ giving the best performance within the investigated range.

3.10 Influence of work function

Investigating the back contact is crucial because its work function, energy-level alignment, and interfacial contact directly influence carrier extraction, contact resistance, interfacial recombination, which in turn affects photovoltaic metrics. This is particularly important for carbon-electrode PSCs, where inefficient charge transfer at the rear interface can limit device performance [12, 13]. The rear-contact work function strongly affects the photovoltaic performance of the CsFAMAPbIBr PSC. Increasing the work function from 4.50 eV to 5.00 eV increases V_{OC} from 0.93 to 1.24 V, J_{SC} from 20.85 to 21.47 mA/cm^2 , and FF from 60.60 to 74.79% (Table 7), resulting in a substantial increase in PCE from 11.78 to 19.91%. The pronounced changes in V_{OC} and FF show that rear-contact energy alignment play an important role in voltage preservation and hole extraction.

Cu_2O is p-type, therefore, increasing the rear-contact work function reduces the energy barrier for hole extraction. Under the ideal Schottky-Mott approximation (Eq. 23) [13, 71].

$$\phi_{B,p} = E_g + \chi - \phi_M, \quad 23$$

where $\phi_{B,p}$ is hole barrier height, E_g is bandgap of Cu_2O , χ is electron affinity, and ϕ_M is metal work function of back contact.

Table 7. Variation of photovoltaic metrics with back contact work function

Metal	Work function (eV) [32, 72-74]	V _{OC} (V)	J _{SC} (mA/cm ²)		FF (%)	PCE (%)
Fe	4.50	0.93	20.85	60.60	11.78	11.78
Mo	4.60	1.03	21.01	62.53	13.56	13.56
Cu	4.65	1.08	21.08	63.23	14.44	14.44
C	5.00	1.24	21.47	74.79	19.91	19.91

The increase in V_{OC} can be attributed to the reduction in the hole-extraction barrier and associated contact recombination losses as the rear-contact work function increases [75]. At lower work functions, the larger barrier promotes carrier accumulation near the Cu₂O/contact interface, increasing recombination and limiting the photovoltage. A higher work function facilitates hole transfer and reduces these voltage losses, thereby increasing V_{OC}.

The increase in FF can be attributed to improved hole extraction and lower contact-related resistance. Reducing the rear-contact barrier decreases the voltage loss during current flow and improves the squareness of the J-V curve [76]. The comparatively small increase in J_{SC} can be ascribed to improved carrier collection because the rear-contact work function does not directly alter light absorption in the CsFAMAPbIBr absorber.

3.11 Error margins and sensitivity

The error-margin and sensitivity analyses are used to identify which device parameters most strongly control the PCE and, consequently, which parameters require the tightest fabrication control [13]. The error margin and sensitivity are expressed according to Eqs. 24 & 25 [13, 77]. A high sensitivity value indicates that device performance is strongly affected by variation in a given parameter, whereas a low sensitivity signifies greater tolerance.

$$\text{Error margin (E}_m\text{)} = \left(\frac{\eta_{\text{max}} - \eta_{\text{min}}}{\text{PCE}_{\text{max}}} \right) \times 100 \quad 24$$

$$\text{Sensitivity (S)} = \frac{E_m}{100} \quad 25$$

where η_{max} is maximum PCE, and η_{min} minimum PCE.

Table 8 reveals that the CsFAMAPbIBr bulk defect density is the most influential parameter, with an error margin of 71.25% and sensitivity of 0.713. This explains why an increase in the defect density reduces the PCE from 21.01 to 6.04%. This result identifies absorber defect suppression and passivation as the most important requirements for maintaining high device efficiency. Shunt resistance is the second most sensitive parameter, with sensitivity of 0.515. This explains the increase in PCE with rising shunt resistance. Therefore, minimizing pinholes, shunting paths and poorly isolated interfaces is essential for preserving a high FF and PCE.

Table. 8. Sensitivity and error margins for the various parameters

Parameter varied	Range tested	PCE (%)		Error margin (%)	Sensitivity	Sensitivity class
		Max.	Min.			
Thickness of BaSnO ₃ (μm)	0.02-0.06	19.85	19.64	1.06	0.011	Very low
Thickness of Absorber (μm)	0.5-0.9	21.23	19.18	9.66	0.097	Very low
Thickness of Cu ₂ O (μm)	0.2-0.6	19.93	19.91	0.10	0.001	Very low
Carrier concentration in BaSnO ₃ (cm ⁻³)	10 ¹⁴ - 10 ¹⁷	19.97	19.90	0.35	0.004	Very low
Carrier concentration in Absorber (cm ⁻³)	10 ¹³ - 10 ¹⁶	19.91	18.61	6.53	0.065	Very low
Carrier concentration in Cu ₂ O (cm ⁻³)	10 ¹⁴ - 10 ¹⁸	21.62	19.74	8.70	0.087	Very low
Defect density of BaSnO ₃ (cm ⁻³)	10 ¹⁴ - 10 ¹⁸	19.91	19.64	1.36	0.014	Very low
Defect density of Absorber (cm ⁻³)	10 ¹⁴ - 10 ¹⁸	21.01	6.04	71.25	0.713	High
Defect density of Cu ₂ O (cm ⁻³)	10 ¹⁴ - 10 ¹⁸	19.91	19.58	1.66	0.017	Very low
Interface defect density of BaSnO ₃ /Absorber (cm ⁻²)	10 ¹⁰ - 10 ¹⁴	19.92	19.35	2.86	0.029	Very low
Interface defect density of Absorber/Cu ₂ O (cm ⁻²)	10 ¹⁰ - 10 ¹⁴	22.14	18.24	17.62	0.176	Low

Bandgap (eV)	1.60-1.68	19.91	17.40	12.61	0.126	Low
Series resistance (Ωcm^2)	1-4	19.58	18.60	5.01	0.050	Very low
Shunt resistance (Ωcm^2)	10^2 - 10^5	19.90	9.66	51.46	0.515	High
HighWork function (eV)	4.50=5.00	19.91	11.78	40.83	0.408	Moderate

The back-contact work function has a moderate influence ($S=0.408$), with higher work function improving Cu_2O /contact alignment, which reduces the hole-extraction barrier and increases PCE from 11.78 to 19.91%. The $\text{CsFAMAPbIBr}/\text{Cu}_2\text{O}$ interface is more sensitive to defects ($S=0.176$) than the BaSnO_3 /absorber interface ($S=0.029$), indicating the importance of rear-interface passivation. The absorber bandgap has relatively low sensitivity ($S=0.126$), reflecting the trade-off between V_{OC} and J_{SC} . In contrast, layer thicknesses, bulk defects in the transport layers, carrier concentrations and series resistance show very low sensitivity.

3.12 Performance of the optimized PSC

The optimized device is simulated using the values in Table 6. These optimal input parameters are supported by previous experimental works on PCS to ensure an optimized device performance that is close to a practical device.

Table 9. Optimal parameters for simulating of the optimized cell

Optimal parameters	BaSnO_3	Absorber	Cu_2O	Reference
Thickness (μm)	0.02	0.9	0.6	-
N_{D} (cm^{-3})	10^{17}	-	-	-
N_{A} (cm^{-3})	[14, 15]	10^{16}	10^{18} [16, 17]	
Bulk defect density, N_{t} (cm^{-3})	10^{14}	10^{14}	10^{14}	[20, 21]
Interface defect, N_{it} (cm^{-2})		10^{10}		[22, 23]
Series resistance (Ωcm^2)		1		[24]

Shunt resistance (Ωcm^2)	10^5	[19, 25]
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Fig. 12 summarizes the electrical and spectral behaviour of the optimized FTO/BaSnO₃/CsFAMAPbIBr/Cu₂O/C device. The J-V (Fig. 12) characteristic shows a high J_{SC} (23.90 mA/cm²), which gives V_{OC} , FF and PCE of 1.32 V, 85.23%, and 26.97%, respectively. The large V_{OC} indicates that recombination losses have been strongly suppressed, allowing a large separation of the electron and hole quasi-Fermi levels under illumination. Meanwhile, the high FF indicate efficient carrier extraction with limited parasitic voltage and current losses. This behaviour agrees with the optimal values of R_s (1 Ωcm^2) and R_{sh} ($10^5 \Omega\text{cm}^2$). The low R_s minimizes the internal voltage drop (JR_s) near the maximum-power region, whereas the high R_{sh} restricts leakage pathways that would reduce the squareness of the J-V curve. The low bulk defect density of 10^{14} cm^{-3} and interface defect density of 10^{10} cm^{-2} further suppressed Shockley-Read-Hall recombination, thereby supporting both the high V_{OC} and FF. Interestingly, the V_{OC} and PCE is consistent with Shockley-Queisser limit of 1.31 eV and 30.14%, respectively, for an absorber with bandgap of 1.6 eV [78].

The near unity QE spectrum (Fig. 12b) supports the high J_{SC} , indicating that harvesting of incident photons, carrier generation, and extraction of the transport layers. The QE decreases toward longer wavelengths, because the photon energy approaches the absorber bandgap and the absorption coefficient becomes smaller.

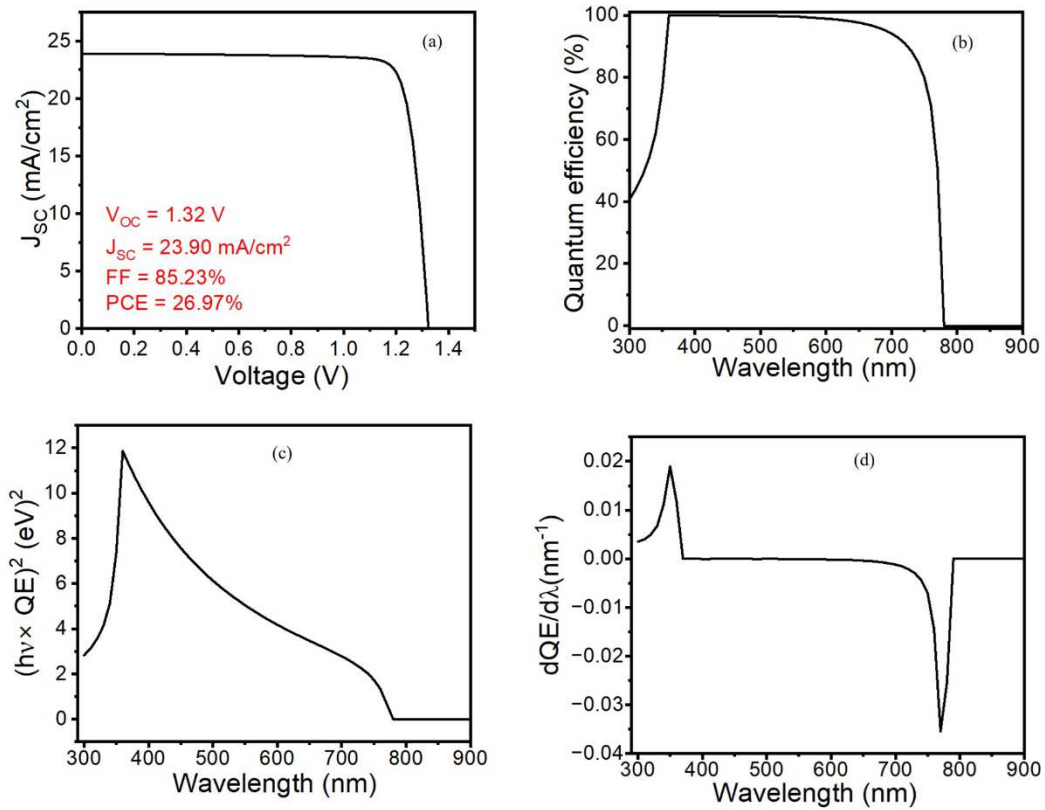


Fig. 12. (a) J-V characteristic of the optimized cell, (b) Associated QE spectrum, (c) Graph of $(h\nu \times QE)^2$ vs. wavelength, (d) $dQE/d\lambda$ vs. wavelength.

The transformed spectral response (Fig. 12c) provides an additional view of the absorption-edge region. The pronounced decrease toward longer wavelength indicates the progressive reduction in usable photon energy and carrier generation as photon energy approaches the electronic transition threshold. This spectral edge is more clearly resolved by the derivative $dQE/d\lambda$ (Fig. 12d). The strong negative minimum near ~ 775 nm corresponds to the wavelength where QE decreases most rapidly (i.e., the inflection points of the absorption edge). This agrees very well with the 1.60 eV bandgap of the absorber. The agreement between the imposed absorber bandgap and the independently observed QE cut-off confirms the internal consistency of the simulated optical and electrical responses.

3.12.1 Carrier generation and recombination profiles

Fig. 13a shows the spatial distribution of photocarrier generation across the optimized FTO/BaSnO₃/CsFAMAPbIBr/Cu₂O/C PSC. The generation rate rises sharply in the absorber (at 0.52 μm) and reaches a maximum of $(8.88 \times 10^{21} \text{ cm}^{-3}\text{s}^{-1})$. It then decreases continuously toward the rear interface. This profile agrees with the Beer-Lambert attenuation of the incident photon flux, which states that the photon density is highest at the front of the absorber, while progressive optical absorption reduces the number of photons available for carrier generation deeper inside the film [79]. The near-zero generation within the transport layers confirms that useful photogeneration occurs predominantly in the CsFAMAPbIBr absorber layer.

Fig. 13b demonstrates that recombination is comparatively low through most of the absorber but increases toward its rear region and produces a narrow maximum of $\sim 1.64 \times 10^{20} \text{ cm}^{-3}\text{s}^{-1}$ at 1.40 μm at the back of the absorber. The localized peak arises because photogenerated holes are extracted toward Cu₂O while minority electrons are blocked from entering the HTL, which produces enhanced electron-hole population overlap near the heterointerface. The moderate optimized interface defect density, and absorber bulk defect density limits recombination throughout most of the active layer. Importantly, the interfacial recombination peak is narrow and spatially localized, whereas the absorber maintains a high generation rate over a much broader region. The maximum generation rate is also about 50 times larger than the maximum recombination rate. Although the peak values alone should not be interpreted as the total generated and recombined carrier populations, the large separation between their magnitudes and the low bulk recombination indicate that most photogenerated carriers are available for extraction without being lost through non-radiative processes. This behaviour is consistent with the high QE and PCE of 26.97%.

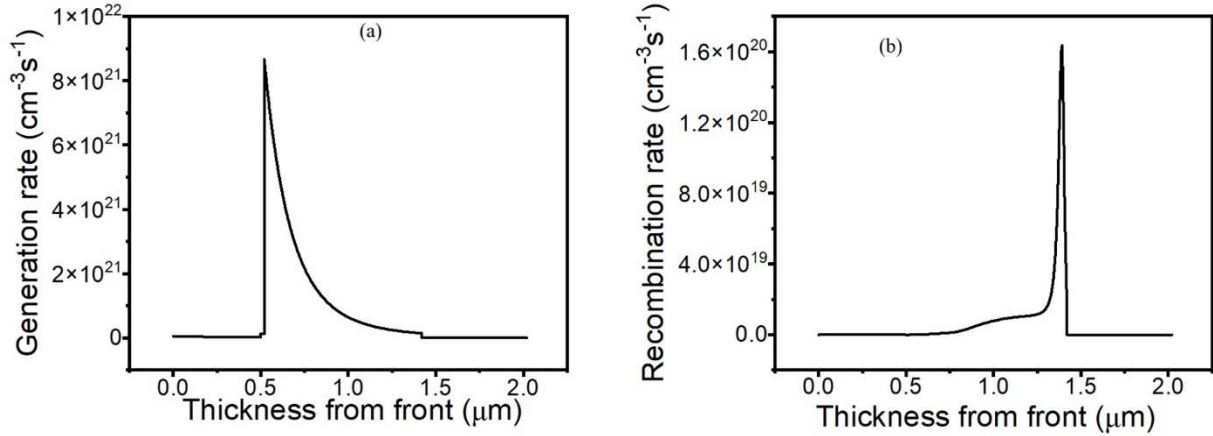


Fig. 13. Carrier generation rate of the optimized cell, (b) Recombination profile.

3.12.2 Performance comparison of the current results with previous related works

Table 10 compares the optimized FTO/BaSnO₃/CsFAMAPbIBr/Cu₂O/C PSC with previously reported experimental and simulated works on CsFAMAPbIBr. The present carbon back-contact device achieves high performance metrics. The PCE is substantially higher than the experimental devices (Table 10), whose PCEs range from 16.01% to 22.37%.

An important feature of this comparison is that the improvement in the present device does not originate from an unusually large photocurrent. Its J_{SC} of 23.90 mA/cm² is comparable with experimental values of 23.95 and 24.00 mA/cm² [9, 80, 81]. The major advantage is the simultaneous increase in V_{OC} (1.32 V) and FF (85.23%), which exceeds the 0.958–1.22 V and 73–82% range of the experimental devices. Physically, this indicates that the principal PCE gain arises from reduced non-radiative recombination, improved quasi-Fermi-level splitting, better carrier selectivity and lower resistive losses.

Compared with previous simulations, the present PCE of 26.97% also exceeds the 17.92–21.94% obtained for ITO/SnO₂/CsFAMAPbIBr/Spiro-OMeTAD/Au structures. However, it remains slightly below the simulated values of 28.01%, 28.66% and 29.08% reported for Ag- or Au-contacted architectures. This difference is physically reasonable because Au and Ag generally provide highly conductive contacts and favourable contact energetics. It should be noted that the significance of the present result is not that it gives the highest simulated PCE, but that a competitive efficiency of 26.97% is obtained while retaining a low-cost carbon as the rear electrode. The merit of the current study is that it retains finite series and shunt resistances together

with realistic bulk and interface defect densities instead of assuming an ideal loss-free device. Therefore, the modest difference between the present PCE of 26.97% and the higher simulated literature values of 28–29% represents a reasonable trade-off for a device architecture that is potentially cheaper, more scalable and more fabrication-oriented.

Table 10. Comparison of photovoltaic performance between the present results and previous CsFAMAPbIBr-based PSCs

Solar cell structure	Method of preparation	Bandgap of perovskite layer (eV)	V _{OC} (V)	J _{SC} (mA/cm ²)	FF (%)	PCE (%)	Ref.
FTO/BaSnO ₃ /CsFAMAPbIBr/Cu ₂ O/C	SCAPS-1D	1.60	1.32	23.90	85.23	26.97	This work
FTO/ZnO/CsFAMAPbIBr/CBTS/Au	SCAPS-1D	1.60	1.37	23.86	88.79	29.08	[13]
FTO/Li-SnO ₂ /CsFAMAPbIBr/Spiro-MeOTAD/Au.	Experiment	1.56	0.958	22.89	73.03	16.01	[82]
FTO/SnO ₂ /CsFAMAPbIBr/Spiro-MeOTAD/Au	Experiment	1.50	1.07	24.00	76.3	20.01	[9]
FTO/TiO ₂ /Cs _x (MA _{0.17} FA _{0.83}) _{1-x} Pb(I _{0.83} Br _{0.17}) ₃ /CuSCN/Au	SCAPS-1D	1.48	1.48	23.27	83.18	28.66	[80]
ITO/PCBM/Cs _{0.05} (FA _{0.77} MA _{0.23}) _{0.95} Pb(I _{0.77} Br _{0.23}) ₃ /CuSbS ₂ /Ag	Experiment	1.67	1.22	20.70	82.00	20.80	[10]
ITO/SnO ₂ /Cs _{0.05} FA _{0.79} MA _{0.15} PbI _{2.45} Br _{0.55} /Spiro-OMeTAD/Au	SCAPS-1D	1.60	1.08	22.297	74.75	17.92	[5]
FTO/TiO ₂ /Li-TiO ₂ /Cs _x (MA _{0.17} FA _{0.83}) _(100-x) Pb(I _{0.83} Br _{0.17}) ₃ /Spiro-OMeTAD/Au	Experiment	1.61	1.13	22.69	74.80	19.20	[6]
ITO/PCBM/Cs _{0.05} (FA _{0.77} MA _{0.23}) _{0.95} Pb(I _{0.77} Br _{0.23}) ₃ /CuSbS ₂ /Ag	SCAPS-1D	1.67	1.12	29.84	83.78	28.01	[10]
FTO/TiO ₂ /Cs _{0.05} (MA _{0.17} FA _{0.83}) _{0.95} Pb(I _{0.83} Br _{0.17}) ₃ /Spiro-OMeTAD/Au	Experiment	1.63	1.14	22.60	0.758	19.61	[7]
FTO/SnO ₂ /CsFAMAPbIBr/Spiro-OMeTAD/Au	Experiment	-	-	-	-	22.37	[67]
FTO/Li-SnO ₂ /CsFAMAPbIBr/Spiro-MeOTAD/Au	Experiment	1.60	1.010	23.95	81.47	19.70	[81]

3.13 Thermal stability test under varying temperature

The operating temperature of PSC is evaluated because temperature directly influences carrier recombination, quasi-Fermi-level splitting, V_{OC} , FF and overall PCE, while repeated thermal exposure can additionally induce strain, phase transitions and ion-related instability under practical operating conditions [83, 84]. The influence of operating temperature on the optimized PSC shows that the photovoltaic response is determined by the temperature dependence of V_{OC} . V_{OC} decreases from 1.34 to 1.29 V as temperature increases from 290 to 330 K (Fig. 14), corresponding to a temperature coefficient of approximately -1.25 mVK^{-1} . In contrast, J_{SC} remains essentially unchanged at $23.90\text{--}23.91 \text{ mA/cm}^2$. As a result, the PCE decreases from 27.18% to 26.06%, while the FF shows only a small variation from 85.12% to 84.71%.

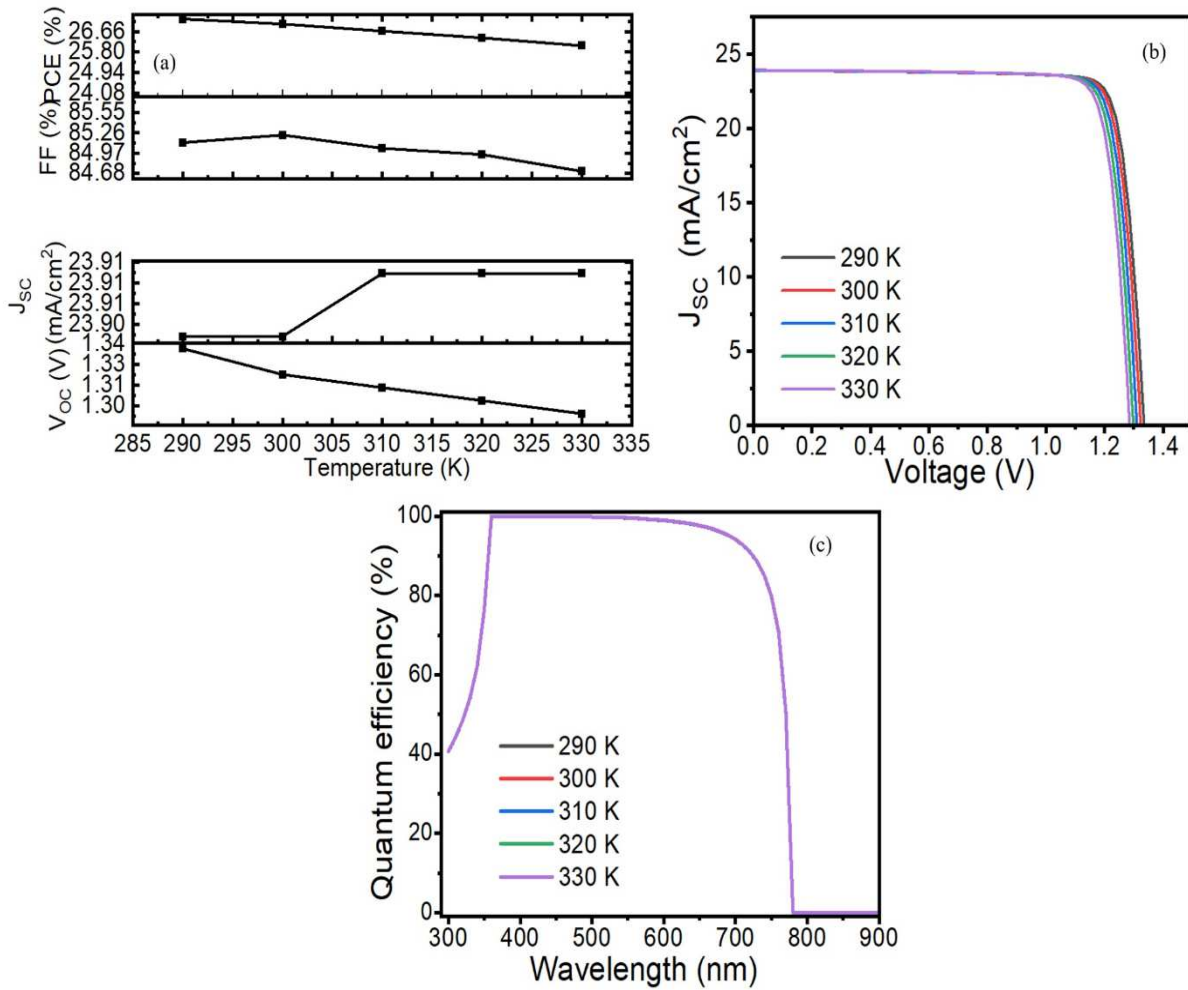


Fig. 14. Variation of VOC, JSC, FF, PCE with temperature.

The reduction in V_{OC} originates primarily from the temperature-induced increase in the diode saturation current and carrier recombination (Eq. 10).

Although the explicit T term increases with temperature, J_0 rises much more strongly because carrier activation and recombination become more pronounced (Eq. 26), where k_B is Boltzmann constant [83].

$$J_0 \propto T^3 \exp\left(\frac{E_g}{k_B T}\right). \quad 26$$

Eq. 26 holds that an increase temperature increases the dark recombination current, reduces electron-hole quasi-Fermi-level splitting and consequently lowers V_{OC} . The relatively moderate reduction in V_{OC} over 290–330 K indicates that recombination is reasonably controlled in the optimized device. The almost temperature-independent J_{SC} shows that photogeneration and carrier collection are not significantly affected. The negligible increase from 23.90 to 23.91 mA/cm² may arise from slightly improved thermally assisted carrier transport or minor changes in carrier distribution. The overlapping QE spectra support the essentially constant J_{SC} , suggesting that photon absorption and carrier extraction did not change.

The FF initially increases slightly from 85.12% at 290 K to 85.23% at 300 K, but subsequently decreases to 84.71% at 330 K. The small initial improvement suggests a balance between thermally assisted carrier transport and recombination. At higher temperatures, however, increased recombination and the reduction in normalized V_{OC} begin to dominate (Eq. 27) [85], where v_{oc} is dimensionless.

$$v_{oc} = \frac{qV_{OC}}{nk_B T} \quad 27$$

And the ideal FF approximately follows Eq. 28 [85],

$$FF = \frac{v_{oc} - \ln(v_{oc} + 0.72)}{v_{oc} + 1} \quad 28$$

Therefore, the simultaneous decrease in V_{OC} and increase in T lower v_{oc} , leading to a gradual deterioration of FF at elevated temperature. The reduction in PCE (Eq. 12) from 27.18% at 290 K to 26.06% at 330 K is mainly driven by the loss in V_{OC} , with a smaller contribution from FF, while J_{SC} remains essentially unaffected. The total PCE loss is only about 4.1% relative over a 40 K increase, corresponding to an approximate relative temperature coefficient of $-0.10\% \text{ K}^{-1}$.

4. Conclusion

In summary, this study demonstrates an experimentally realistic route for improving the performance of carbon-electrode-based $\text{Cs}_{0.05}\text{FA}_{0.79}\text{MA}_{0.15}\text{PbI}_{2.45}\text{Br}_{0.55}$ PSCs using SCAPS-1D. Starting from FTO/BaSnO₃/CsFAMAPbIBr/Cu₂O/C architecture, the prototype PSC delivered a PCE of 19.91%, with V_{OC} of 1.24 V, J_{SC} of 21.47 mA/cm² and FF of 74.79%. Systematic optimization of layer thickness, carrier concentration, bulk and interface defect densities, and resistive losses increased the PCE to 26.97%, with V_{OC} of 1.32 V, J_{SC} of 23.90 mA/cm² and FF of 85.23%. The optimized device retained a low-cost carbon back contact and relied on parameter ranges that remain compatible with experimentally attainable materials and processing conditions. Sensitivity analysis identified absorber bulk defect density, shunt resistance and rear-contact work function as the dominant performance-controlling parameters. Meanwhile moderate variations in transport-layer thickness and carrier concentration produced comparatively small changes. The results further show that suppressing non-radiative recombination in the absorber and at the CsFAMAPbIBr/Cu₂O interface, while maintaining low series resistance and high shunt resistance, is critical for sustaining high V_{OC} and FF. Temperature analysis showed that the cell retained a PCE above 26% from 290 to 330 K, indicating modest temperature-induced performance variation. These findings provide practical design guidance for efficient, low-cost triple-cation mixed-halide PSCs and establish a realistic framework for future experimental fabrication and validation.

Statements and Declarations

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Author Contributions

P.R.J.: Conceptualization, Methodology, Investigation, Writing – original draft; **I.A.T.:** Investigation, Writing – original draft **C.A.:** Conceptualization, Methodology; **K.I.U.:** Conceptualization, Methodology; **I.K.N.:** Conceptualization, Methodology; **A.O.A.:** Conceptualization, Methodology, Investigation; **M.M.G.:** Software, Validation; **I.I.A.:** Software;; **A.N.A.:** Writing – Reviewing; **C.A.M.:** Supervision, Validation; **E.E.O.:** Funding acquisition, Supervision, Resources; Validation.

Competing Interests

The authors have no relevant financial or non-financial interests to disclose.

Data Availability

The data supporting the findings of this study are available from the corresponding author **upon** reasonable request.

Code Availability

No custom code was developed for this study. Numerical simulations were performed using SCAPS-1D.

Ethics Approval

Not applicable.

Consent to Participate

Not applicable.

Consent for Publication

Not applicable.

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