
Research article

Influence of MAPbI₃ absorber layer properties on WO₃/MAPbI₃/GO perovskite solar cells' performance using SCAPS-1D

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Abstract: The solar cell capacitance simulator in one dimension was used to examine how the perovskite layer's properties influence devices' performance in a simulated solar cell structure comprising graphene oxide (GO) as the hole transport material (HTL), tungsten trioxide (WO₃) as the electron transport material (ETL), and methylammonium lead iodide (MAPbI₃) as the absorber layer. The simulation investigated the effects of the MAPbI₃ layer's thickness, defect density, electron affinity, and doping concentration on photovoltaic parameters. The baseline nonoptimized structure yielded a power conversion efficiency (PCE) of 7.1%, with a short-circuit current density (J_{sc}) of 11.38 mA/cm², an open-circuit voltage (V_{oc}) of 0.80 V, and a fill factor (FF) of 77.9%. Optimization of the MAPbI₃ layer's thickness to 1.2 μm and the acceptor doping density to 1.0 × 10²² cm⁻³ improved the PCE to 22.9%, with J_{sc} = 28 mA/cm², V_{oc} = 0.93 V, and FF = 87.4%. These improvements stem from enhanced light absorption and more efficient charge separation. Alternating current (AC) analysis through capacitance–voltage and electrochemical impedance spectroscopy indicated that optimized doping reduces series resistance and modifies the depletion

region's width, though the interpretation of the Nyquist plots requires careful consideration of competing transport and recombination processes. These findings provide guidance for experimental design of perovskite solar cells, though the simulated efficiencies represent theoretical upper bounds that may not be achievable experimentally with these transport layer materials.

Keywords: perovskite solar cells; MAPbI₃; graphene oxide; tungsten trioxide; SCAPS-1D simulation; doping optimization

1. Introduction

The rapid consumption of fossil fuels over recent decades has precipitated energy resource depletion, environmental degradation, and rising costs. Consequently, research has intensified toward sustainable energy technologies with reduced environmental impact [1]. Solar energy conversion represents one of the most viable alternatives, with photovoltaic technology advancing through the development of new materials and device architectures [2,3]. The first silicon solar cell, fabricated by Chapin and colleagues in 1954, achieved 6% power conversion efficiency [4]. While silicon technology remains dominant, the high processing costs and energy-intensive manufacturing have motivated investigation of alternative absorber materials. Organic–inorganic hybrid perovskite solar cells (PSCs), particularly those based on methylammonium lead iodide (MAPbI₃), have emerged as promising candidates due to their high absorption coefficients, long carrier diffusion lengths, and solution processability [5–7].

MAPbI₃ continues to serve as a reference material in perovskite research, possessing a bandgap of approximately 1.55 eV that is suitable for single-junction solar cells, and demonstrating power conversion efficiencies exceeding 22% in optimized laboratory devices [8]. Compared with formamidinium-based or mixed-cation perovskites, MAPbI₃ offers simpler processing and greater reproducibility, though with somewhat reduced thermal stability [9].

A typical PSC comprises three functional layers: The hole transport layer (HTL), the electron transport layer (ETL), and the absorber perovskite layer. The HTL collects photogenerated holes and blocks electrons, while the ETL performs the complementary function for electrons. The efficiency of these transport layers critically determines overall device performance [10,11]. Traditional organic transport materials, while processable at low temperatures, often suffer from limited stability and modest charge carrier mobilities [12]. Inorganic metal oxides have attracted attention as alternatives, with WO₃ investigated as an ETL due to its suitable conduction band position, optical transparency, and chemical stability [13–16]. Graphene oxide (GO) has been examined as an HTL or interface modifier owing to its solution processability and electron-blocking properties, though its intrinsic hole conductivity remains limited [17]. Recent work has explored engineering the hole transport interface directly, for example, using a star-shaped nitrogen-rich small-molecule interlayer to improve hole extraction and device performance [18].

This study presents a computational investigation of a WO₃/MAPbI₃/GO device structure using solar cell capacitance simulator in one dimension (SCAPS-1D) simulation software. The work focuses specifically on how variations in the MAPbI₃ layer's properties, namely its thickness, doping concentration, defect density, electron affinity, and bandgap, affect the direct current (DC)

photovoltaic parameters and alternating current (AC) impedance characteristics. The objective is to identify the optimal absorber layer conditions and to examine whether the chosen transport layer combination can support high-efficiency operation.

2. Theoretical background

Band alignment and heterojunction physics

The performance of multilayer PSCs is strongly influenced by the energy level alignment at the interfaces between the absorber and charge transport layers. The conduction band offset (CBO) and valence band offset (VBO) determine the carrier extraction and recombination behavior. These offsets are defined as

$$\Delta E_c = \chi_{\text{absorber}} - \chi_{\text{ETL}}, \Delta E_v = (E_{g,\text{HTL}} - \chi_{\text{HTL}}) - (E_{g,\text{absorber}} - \chi_{\text{absorber}}) \quad (1)$$

where χ is the electron affinity and E_g is the bandgap of the respective layers. Spike-like conduction band offsets ($\Delta E_c > 0$) can enhance electron confinement but may hinder extraction if the barrier exceeds the thermal energy of the carriers, whereas cliff-like offsets ($\Delta E_c < 0$) facilitate extraction but may increase interfacial recombination. For the $\text{WO}_3/\text{MAPbI}_3/\text{GO}$ system, typical offsets of $\Delta E_c \approx 0.3$ eV and $\Delta E_v > 3$ eV promote selective charge transport while minimizing carrier losses at the interfaces.

Recombination mechanisms

The V_{oc} of PSCs is limited by recombination processes. In the bulk of the absorber, Shockley–Read–Hall (SRH) recombination dominates in the presence of trap states when the defect density satisfies

$$N_t > \frac{1}{\sigma v_{th} \tau_{rad}} \quad (2)$$

where σ is the capture cross-section, v_{th} is the thermal velocity, and τ_{rad} is the radiative lifetime. At interfaces, recombination is controlled by the density of the interface states and local band bending, which governs carrier concentrations. At high carrier densities, radiative and Auger recombination also contribute significantly. The V_{oc} can be approximated as

$$V_{oc} \approx \frac{kT}{q} \ln \left(\frac{J_{sc}}{J_0} + 1 \right) \quad (3)$$

where J_0 is the dark saturation current, J_{sc} is the short-circuit current density, k is Boltzmann's constant, T is the temperature, and q is the elementary charge.

Drift-diffusion transport

Carrier transport in thin-film PSCs is modeled using the coupled Poisson and continuity equations in one dimension. The Poisson equation relates the electrostatic potential ψ to the spatial distribution of charges

$$\frac{d^2\psi}{dx^2} = \frac{q}{\epsilon_0\epsilon} [p(x) - n(x) + N_D^+ - N_A^-] \quad (4)$$

where n and p are the electron and hole densities, N_D^+ and N_A^- are the ionized donor and acceptor densities, ε_0 is the vacuum permittivity, and ε is the relative dielectric constant. The continuity equations for electrons and holes are given by

$$\frac{dJ_n}{dx} = q(G_{\text{op}} - R(x)), \frac{dJ_p}{dx} = -q(G_{\text{op}} - R(x)) \quad (5)$$

where J_n and J_p are the electron and hole current densities, G_{op} is the optical generation rate, and $R(x)$ is the net recombination rate. Currents include the drift and diffusion contributions

$$J_n = q\mu_n n \frac{d\psi}{dx} + qD_n \frac{dn}{dx}, J_p = q\mu_p p \frac{d\psi}{dx} - qD_p \frac{dp}{dx} \quad (6)$$

with μ and D representing carrier mobilities and diffusion coefficients, respectively. Steady-state transport with Ohmic contacts is typically assumed.

Transport layer selectionlayer selection

The choice of transport layers critically affects carriers' extraction and recombination. In this study, the ETL is stoichiometric, donor-doped n-type tungsten trioxide (WO_3), with the parameters listed in Table 1. WO_3 is selected because of its high electron affinity (~ 4 eV), chemical stability, and favorable conduction-band alignment with the MAPbI_3 absorber. It differs from the oxygen-deficient WO_x produced by thermal evaporation, which may exhibit p-type behavior and different energy levels. Experimentally, stoichiometric WO_3 can be deposited by reactive magnetron sputtering in a controlled Ar/O_2 atmosphere, followed by annealing in air or oxygen [19,20]. Its stoichiometry and oxidation state can be verified using X-ray photoelectron spectroscopy. Therefore, this study describes an idealized n-type WO_3 ETL and does not assume that thermally evaporated p-type WO_x has the same energy band diagram. GO serves as the HTL [17,21], offering a valence band alignment suitable for efficient hole extraction and a large conduction band offset to block electrons. Partial reduction of GO further tunes its work function and conductivity, improving interfacial contact and minimizing recombination losses.

Figures of merit

The photovoltaic performance is evaluated using standard figures of merit. The PCE (η) is given by

$$\eta = \frac{J_{\text{sc}} V_{\text{oc}} \text{FF}}{P_{\text{in}}} \quad (7)$$

where J_{sc} is the short-circuit current density, V_{oc} is the open-circuit voltage, FF is the fill factor, and P_{in} is the incident optical power. J_{sc} depends on light absorption and carrier collection, V_{oc} reflects the quasi-Fermi level splitting under illumination, and FF is influenced by series resistance, recombination, and interfacial quality.

3. Methodology

Device structure

The simulated device consists of fluorine-doped tin oxide (FTO) front contact/ WO_3 ETL (0.20 μm)/ MAPbI_3 (variable thickness)/GO HTL (0.20 μm)/Au back contact. Figure 1 shows the schematic band alignment.

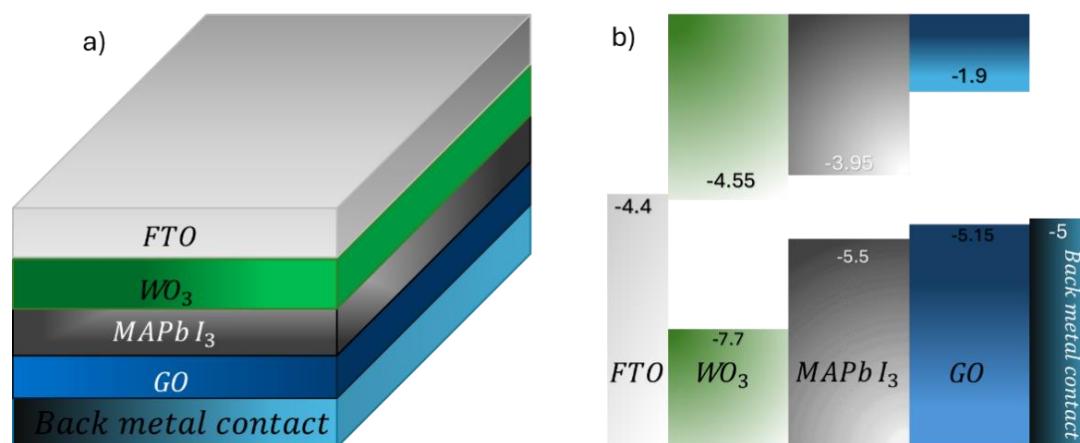


Figure 1. Schematic diagram and energy level alignment of the PSC.

Electrode selection

Au and FTO were selected as the back and front contacts, respectively, on the basis of their work functions and established use in PSC simulation studies. FTO (work function = ~ 4.4 eV) is the standard transparent conducting oxide for the illuminated front contact in SCAPS-1D perovskite device models, providing high optical transmittance combined with adequate conductivity [22].

Au (work function = ~ 5.1 eV) was chosen for the back contact because a high-work-function metal is required to form a quasi-Ohmic contact with the GO HTL and minimize the back-contact barrier for hole extraction; systematic SCAPS-1D studies of back-contact metals in PSCs have shown that device performance is highly sensitive to this work function, with higher-work-function contacts (e.g., Au, Pt) consistently outperforming lower-work-function alternatives (e.g., Ag, Cu, Ni) for hole-extracting back contacts [23].

Simulated device structure and input parameters

SCAPS-1D is a numerical simulation tool developed at the University of Gent, Belgium, for modeling semiconductor-based photovoltaic devices [24,25]. The software solves the coupled Poisson equation and continuity equations for electrons and holes

$$\frac{d^2\psi}{dx^2} + \frac{q}{\epsilon_0\epsilon} [p(x) - n(x) + N_D - N_A + \rho_p - \rho_n] = 0 \quad (8)$$

$$\frac{1}{q} \frac{dJ_p}{dx} = G_{op} - R(x) \quad (9)$$

$$\frac{1}{q} \frac{dJ_n}{dx} = -G_{op} + R(x) \quad (10)$$

where ε is the dielectric constant, q is the electron charge, N_A and N_D are the ionized acceptors and donor density, Ψ is the electrostatic potential, J_p is the current density due to holes, J_n is the current density due to electrons, G_{op} is the carrier generation rate, $R(X)$ is the total recombination rate, P is the free hole density, n is the free electron density, and ρ_p and ρ_n are the hole and electron distributions, respectively. The drift diffusion Eqs (9) and (10) represent the hole and electron carrier transport properties of the semiconducting material. To evaluate the performance of the photovoltaic cells, several key parameters were considered: FF, short-circuit current density (J_{sc}), V_{oc} , and PCE .

Input parameters

Tables 1–3 list the material parameters used in the simulations, selected from published literature values [26,27]. Several parameters warrant discussion: The electron affinity of MAPbI₃ was set to 3.90 eV, consistent with ultraviolet photoelectron spectroscopy measurements, though this value varies in the literature between 3.8 and 4.0 eV depending on measurement technique and film processing [28].

Table 1. Simulation parameters of each layer of the proposed solar cell.

Material characteristics	WO ₃	MAPbI ₃	GO
Thickness of each material (μm)	0.20	Variable	0.20
Bandgap of the material (eV)	3.15	1.55	3.25
Material electron affinity (eV)	4.20	3.90	2.50
Dielectric permittivity of the material (relative)	10	6.5	3.0
Conduction band effective density of states (cm ⁻³)	4.2×10^{18}	2.0×10^{18}	2.2×10^{22}
Valence band effective density of states (cm ⁻³)	9.0×10^{18}	2.0×10^{18}	1.8×10^{21}
Electron mobility (cm ² •Vs ⁻¹)	20	2.0	10
Hole mobility (cm ² •(Vs) ⁻¹)	10	2.0	1
Shallow uniform donor density N _D (cm ⁻³)	1.0×10^{18}	Variable	0
Shallow uniform acceptor density N _A (cm ⁻³)	0	Variable	1.0×10^{16}
Defect density N _t (cm ⁻³)	1.0×10^{15}	Variable	1.0×10^{14}

Note: The electron affinity of GO was adjusted from typical literature values to 2.50 eV to approximate the partial reduction and improved hole extraction in processed films.

The doping concentrations represent the effective carrier densities under illumination rather than equilibrium values, as MAPbI₃ typically exhibits intrinsic behavior with background doping in the 10¹⁴–10¹⁶ cm⁻³ range. With the help of SCAPS-1D software, we understood the influence of various factors that affect the performance of the designed PSC device, including the thickness of the MAPbI₃ layer, doping density, defect density, and electron affinity. Optimizing these factors leads to a significant improvement in the overall output of the PSC, as quantified by V_{oc} , J_{sc} , FF%, and PCE%.

Table 2. Simulation parameters of the back and front contacts of the proposed device.

Parameter	Back contact (<i>Au</i>)	Front contact (<i>FTO</i>)
Surface recombination velocity of electrons ($\text{cm}\cdot\text{s}^{-1}$)	1.0×10^5	1.0×10^7
Surface recombination velocity of holes ($\text{cm}\cdot\text{s}^{-1}$)	1.0×10^7	1.0×10^5
Metal work function (eV)	5.10	4.40

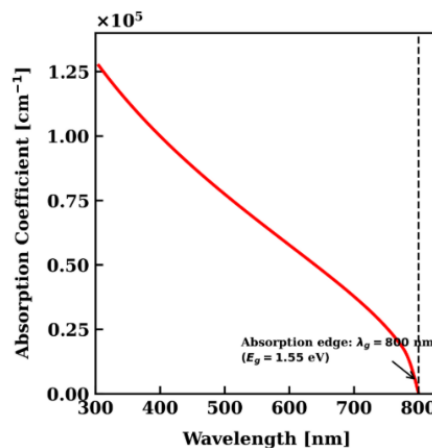
Table 3. Interface defect parameters for GO/MAPbI₃ and MAPbI₃/WO₃ heterojunctions.

Interface	GO/MAPbI ₃	MAPbI ₃ /WO ₃
Defect type	Neutral	Neutral
Energetic distribution	Single level	Single level
Capture cross-section for electrons (cm^{-2})	1.0×10^{-15}	1.0×10^{-15}
Capture cross-section for holes (cm^{-2})	1.0×10^{-15}	1.0×10^{-15}
Reference for defect energy level	Above valence band maximum	Above valence band maximum
Energy of the reference eV	0.60	0.60
Total density (cm^{-3})	1.0×10^{12}	1.0×10^{12}

Simulation conditions

All simulations were performed under AM1.5G illumination ($100 \text{ mW}/\text{cm}^2$) at 300 K unless otherwise specified. The simulations assume: (i) Uniform material properties within each layer, (ii) no ion migration effects, (iii) no hysteresis in current–voltage characteristics, (iv) ideal optical incoupling without reflection or parasitic absorption losses, and (v) Ohmic contacts with fixed work functions. These assumptions represent idealized conditions that may not fully capture the experimental device’s behavior.

Optical absorption model

**Figure 2.** Wavelength-dependent absorption coefficient of the MAPbI₃ absorber used in the SCAPS-1D simulation.

The wavelength-dependent absorption coefficient of MAPbI₃ was generated using the traditional $\sqrt{2(h\nu - Eg)}$ absorption model implemented in SCAPS-1D. Figure 2 shows the absorption spectrum used in the simulations. The absorption coefficient decreases from approximately $1.27 \times 10^5 \text{ cm}^{-1}$ at 305 nm to zero near 800 nm. The absorption edge is consistent with the adopted bandgap of 1.55 eV.

4. Results and discussion

The initial simulation conditions were established to determine the optimal parameters of solar cells, enabling an accurate performance evaluation and a consistent comparison under varying design and material conditions. The device was modeled with operational temperature of 300 K and an MAPbI₃ absorber layer characterized by a bandgap of 1.55 eV and a thickness of 0.1 μm , a doping density of $1.0 \times 10^{18} \text{ cm}^{-3}$ and a defect density of $1.0 \times 10^{14} \text{ cm}^{-3}$. Under these defined conditions, Figure 3 shows the simulated current density–voltage (J–V) curve under illumination. According to the J–V analysis, the PSC device achieved a V_{oc} of 0.80 V, a J_{sc} of 11.38 mA/cm², an FF of 77.9%, and a PCE of 7.1%. These values are the baseline results for establishing a performance benchmark.

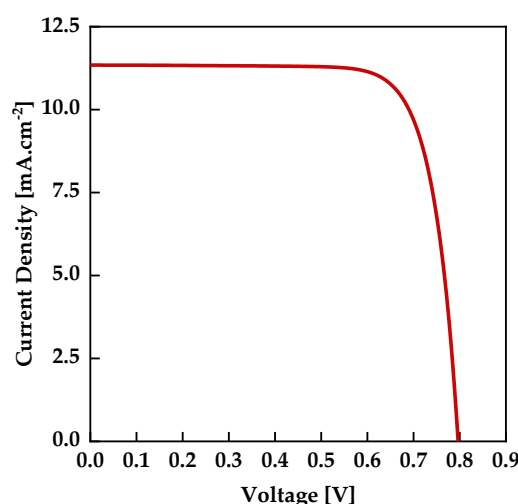


Figure 3. Simulated current density–voltage (J–V) characteristics of the baseline PSC device under standard illumination (AM 1.5G, 100 mW/cm²) at 300 K and a MAPbI₃ thickness of 0.1 μm . The initial device exhibits $V_{oc} = 0.80 \text{ V}$, $J_{sc} = 11.38 \text{ mA/cm}^2$, FF = 77.9%, and PCE = 7.1%.

Perovskite layer optimization

The MAPbI₃ layer was optimized for thickness, doping density, bandgap, electron affinity, and defect density. Calculations were conducted by varying one parameter at a time from the initial set of conditions, while keeping the others constant. Figure 4 shows the effect of the MAPbI₃ layer's thickness on the performance of the PSC device.

The effect of the MAPbI₃ layer's thickness can be explained by the interplay among optical absorption, carrier generation, and the recombination mechanisms [17,29,30]. Figure 4a,b shows that

a change in thickness of the MAPbI₃ layer from 0.1 to 1.5 μm leads to an increase in J_{sc} and PCE from 11.38 mA/cm² to 25.97 mA/cm² and 7.1% to 16.7%, respectively. This agrees with the Beer–Lambert law [31], which states that photon absorption increases with the optical path length, enabling more photogenerated electron–hole pairs. On the other hand, V_{oc} improves from 0.804 V at 0.1 μm to a maximum of approximately 0.838 V around 0.7 μm , which suggests that thicker films initially reduce carrier recombination at the back contact and improve quasi-Fermi level splitting [32,33]. However, beyond approximately 0.7 μm , the V_{oc} declines only marginally, from approximately 0.838 V to 0.835 V at 1.5 μm . This modest decline is consistent with a gradual increase in SRH bulk recombination, as the carriers must travel longer distances before reaching the electrodes, producing a slight decrease in V_{oc} . Similarly, the FF showed a gradual decline from 77.9% to 76.8%, attributed to increased series resistance and reduced charge extraction efficiency in thicker films. PCE reaches a plateau beyond approximately 1.1–1.3 μm , supporting the selection of an absorber thickness near 1.2 μm for the final optimized device.

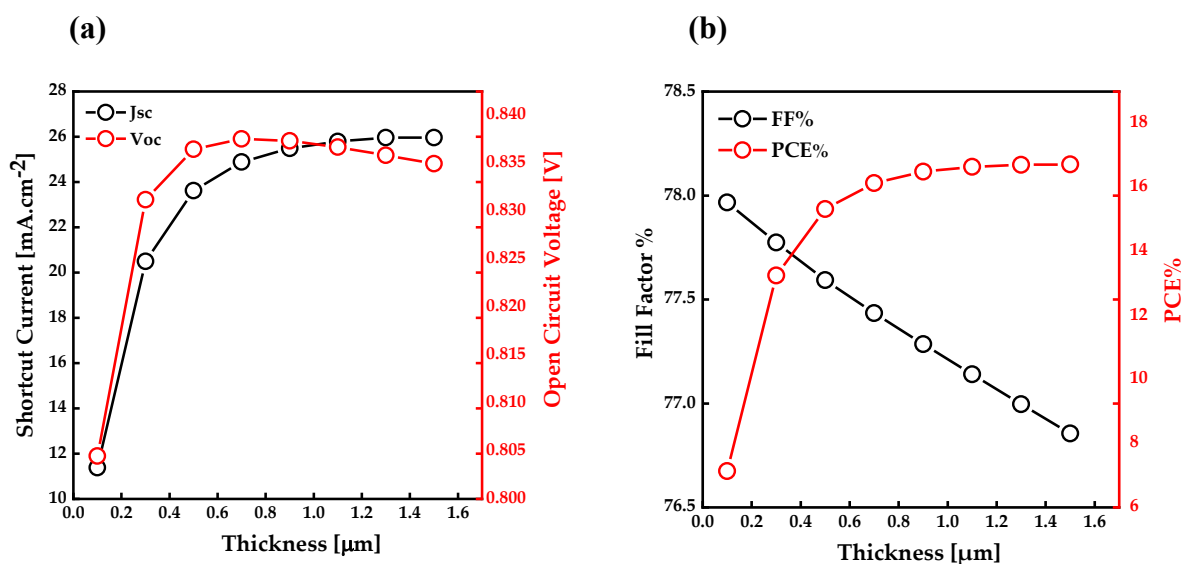


Figure 4. Effect of increasing the MAPbI₃ layer's thickness on (a) J_{sc} and V_{oc} and (b) PCE and FF .

Dopant density impact

Figure 5 shows the effect of the acceptor doping density in the MAPbI₃ layer on the performance of the PSC. The results reveal that the PCE increased steadily with doping density from 7.14% at $1.0 \times 10^{18} \text{ cm}^{-3}$ to 9.37% at $1.0 \times 10^{22} \text{ cm}^{-3}$, while the V_{oc} and FF rose from 0.80 V and 77.97% to 0.96 V and 87.64%, respectively. In contrast, J_{sc} remains nearly unchanged, varying only slightly between 11.38 mA/cm² and 11.16 mA/cm².

These results were attributed to the increase in the free carrier concentration, which reduced the series resistance. Additionally, as the doping density increases, the electric field at the interface becomes stronger, which improves the efficiency of photogenerated carrier separation and extraction. Within the simulated range, V_{oc} and FF continue to improve throughout, though the rate of improvement diminishes markedly beyond approximately $5.0 \times 10^{20} \text{ cm}^{-3}$ – $1.0 \times 10^{22} \text{ cm}^{-3}$, consistent with mobility gains limited by ionized impurity scattering rather than an outright decline. Within this sweep, the best FF and V_{oc} are obtained at the highest tested doping density ($1.0 \times 10^{22} \text{ cm}^{-3}$) [34].

The improvement in FF with increasing doping density reflects the reduction in effective series resistance and the optimization of the depletion region's width. To evaluate the impact of series resistance on the device's performance, a characteristic resistance can be defined as $R_{ch} = V_{oc}/J_{sc}$, which provides a normalization for comparison. High FF values are achieved when the ratio of actual series resistance to characteristic resistance, R_s/R_{ch} , remains below 0.1, a condition that is increasingly well satisfied as the doping density rises across the simulated range. The marked slowdown in FF gains beyond approximately $5 \times 10^{20} \text{ cm}^{-3}$ indicates diminishing returns from further doping increases, likely reflecting the growing influence of ionized impurity scattering on the carrier's mobility. Experimentally, the carrier concentration in MAPbI₃ films can be adjusted through precursor stoichiometry, suitable dopants, and post-deposition annealing. However, achieving very high doping levels while maintaining good film quality and avoiding additional recombination centers is difficult. Therefore, the higher doping concentrations used in this study should be considered mainly as numerical limits rather than easily achievable experimental values. In addition, the absorption spectrum was kept fixed during the doping sweep, so possible changes in optical absorption caused by doping were not included in the simulations

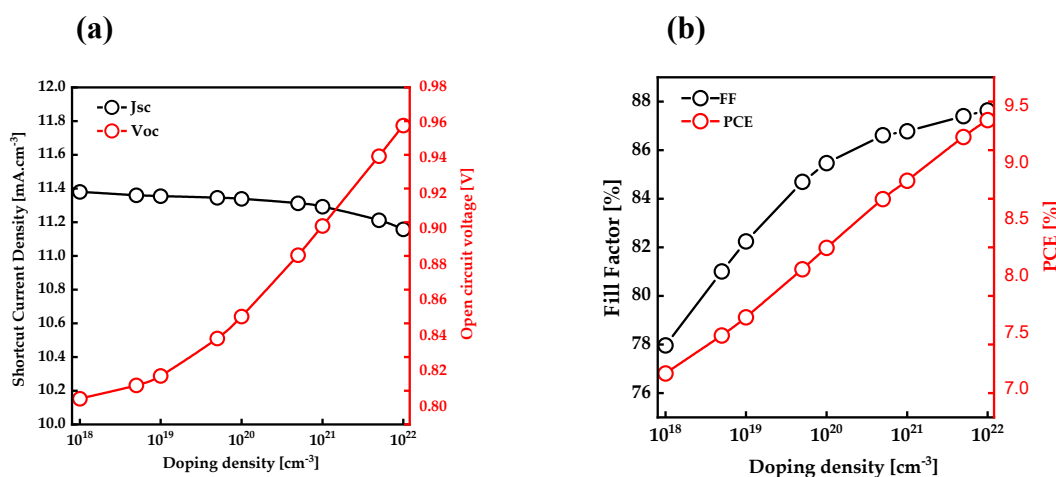


Figure 5. Effect of acceptor doping density in the MAPbI₃ absorber layer on the PSC's performance at 300 K under AM 1.5 G illumination: (a) Variation of J_{sc} and V_{oc} , and (b) corresponding changes in PCE and FF.

On the other hand, the weak doping dependence of J_{sc} can be understood by separating the electrostatics from optical generation. Using the abrupt-junction approximation for the n-WO₃/p-MAPbI₃ interface, $\epsilon_r(\text{WO}_3) = 10$, $\epsilon_r(\text{MAPbI}_3) = 6.5$, $\text{ND}(\text{WO}_3) = 1 \times 10^{18} \text{ cm}^{-3}$, and the built-in potentials extracted from Figure 9 (0.60, 0.65, 0.71, 0.77, and 0.83 V), the calculated total depletion widths are approximately 32.3, 27.4, 28.1, 29.2, and 30.3 nm for MAPbI₃ acceptor densities of 10^{18} , 10^{19} , 10^{20} , 10^{21} , and 10^{22} cm^{-3} , respectively. The corresponding portions extending into MAPbI₃ are approximately 16.2, 2.50, 0.278, 0.029, and 0.003 nm; the sub-nanometer values at $\geq 10^{20} \text{ cm}^{-3}$ signal the breakdown of the continuum depletion approximation and reinforce that these very high densities are numerical sensitivity limits rather than experimentally validated bulk doping levels. The GO-MAPbI₃ contact is p-type-p-type in the adopted parameter set, so a separate

abrupt p–n depletion width is not physically defined there; its band bending is obtained self-consistently by SCAPS-1D from the offsets and interface states. Because the absorption profile and the absorber's thickness are unchanged during the doping sweep, diffusion-assisted collection outside the narrow WO₃/MAPbI₃ space-charge region dominates, and J_{sc} therefore changes only slightly (from 11.38 to 11.16 mA/cm²).

Effect of defect density

The defect density in the MAPbI₃ layer affects the diffusion length and lifetime of charge carriers. Therefore, defect density is considered to be an essential parameter for achieving good performance. Here, the defect density in the MAPbI₃ layer varied from 1.0×10^{12} cm⁻³ to 1.0×10^{21} cm⁻³. Figure 6a shows the change in PCE according to the defect densities. The data show that PCE remains relatively stable at approximately 7.2% for defect density levels up to 1.0×10^{14} cm⁻³. Beyond this threshold, efficiency declines markedly, falling from 6.65% at 1.0×10^{15} cm⁻³ to 0.14% at 1.0×10^{21} cm⁻³. This sharp decline is attributed to the increased defect-mediated recombination, which accelerates the loss of photogenerated charge carriers and consequently reduces the electrical output of the solar cell. An increase in N_t leads to degraded performance characteristics because of the decrease in the carrier's lifetime, which leads to an increase in the recombination rate. The bandgap and electron affinity of the perovskite layer determine the quality of alignment of the energy levels at interfaces created in PSCs [35]. This alignment strongly affects charge extraction, recombination losses, and, ultimately, the device's efficiency. The dependence of device performance on defect density reflects the balance between carrier generation and recombination processes that govern solar cells' operation. The critical transition at $N_t \approx 10^{14}$ cm⁻³ indicates the point at which SRH recombination becomes dominant over radiative recombination. This threshold can be interpreted through the ratio of carrier transit time to the SRH lifetime, expressed as $(\tau_{transit}/\tau_{SRH} = \sigma v_{th} N_t \cdot (\frac{d^2}{2\mu V_{bi}}))$. Efficient charge collection requires this ratio to be less than unity. For the optimized absorber thickness, the carrier's lifetime at the threshold defect density remains long enough to allow complete charge extraction. However, at higher defect densities, the carrier's lifetime becomes shorter than the transit time, leading to severe recombination losses and a rapid degradation in the device's efficiency.

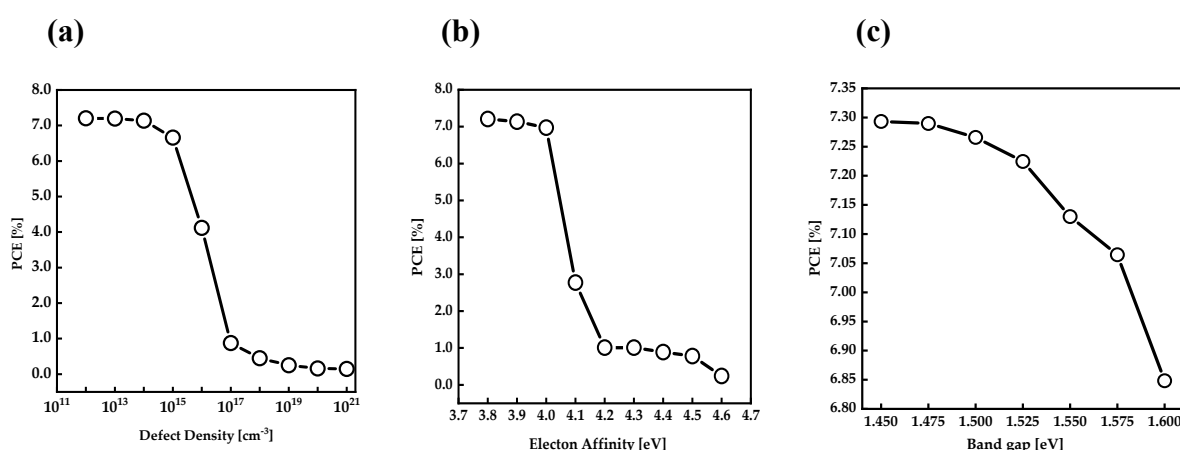


Figure 6. (a) The effect of the defect density in the MAPbI₃ layer. (b) The effect of the electron affinity of the MAPbI₃ layer. (c) The effect of the band gap of the MAPbI₃ layer.

Figure 6b shows the effect of varying the electron affinity of the MAPbI₃ layer from 3.9 eV to 4.6 eV. The results reveal a complex relationship between the electron affinity and the efficiency of the solar cell. The maximum PCE of 7.14% occurs at $\chi = 3.9$ eV because the conduction band of MAPbI₃ aligns optimally with the ETL, enabling efficient electron extraction, minimal recombination, and high J_{sc} . As χ increases beyond 3.9 eV, it creates a barrier for electron flow, reducing the efficiency of solar cells due to misalignment in energy levels between the ETL and the MAPbI₃ layer, which hinders charge extraction and increases recombination, decreasing the PCE to 0.24%. Similar results have been observed in other studies, demonstrating the variation in V_{oc} , J_{sc} , FF, and PCE with conduction band offset (CBO), which affected Cu₂ZnSnS₄ solar cells' performance [36]. Thus, the optimal electron affinity for MAPbI₃ was determined to be 3.9 eV.

Figure 6c shows the effect of varying the band gap (E_g) of the MAPbI₃ from 1.45 eV to 1.60 eV. The results show that the PCE of the device slightly decreases as the E_g of the MAPbI₃ increases from approximately 1.45 eV to 1.52 eV. As E_g increases beyond ~1.52 eV, efficiency began to decline significantly, the decline continuing gradually up to the highest bandgap value simulated (1.60 eV). This decrease was attributed to the reduction in photon absorption and increased recombination losses because a larger E_g can make the energy levels between the absorber and transport layers less aligned, which increases recombination and reduces charge extraction. On the other hand, when we compared the results with our previous report [17], the effect of varying E_g is less significant than in our PSC device. This difference arises from the energy-level alignment between the MAPbI₃ and the ETL.

Temperature dependence

Ambient conditions, including moisture, prolonged light exposure, and temperature fluctuations, significantly affect the stability of solar cells, accelerate degradation, lower efficiency, and shorten the operational lifetime, particularly in PSCs [37,38]. In this section, the effect of temperature on the performance of PSCs is investigated. The results are presented in Table 4 and plotted in Figure 7.

Table 4. Parameters of PSC as a function of temperature.

T (K)	PCE%	FF%	J_{sc} (mA/cm ²)	V_{oc} (V)
280	7.23	78.48	11.38	0.810
300	7.14	77.97	11.38	0.804
320	6.94	76.94	11.38	0.792
340	6.72	75.78	11.39	0.779
360	6.49	74.65	11.39	0.764
380	6.26	73.62	11.39	0.746
400	6.02	72.73	11.40	0.726

According to the literature, when the temperature of solar cells increases, more electron–hole pairs are generated owing to the increased thermal energy, which decreases V_{oc} [38]. However, higher temperatures usually influence the physical and chemical properties of the materials used in solar cells. They cause an expansion of the interatomic spacing in the components of the materials and lead to a reduction in the E_g . This mechanism contributes to the observed decrease in PCE with increasing temperature, and the bonds between the atoms or molecules in the solar cell components are broken at high temperatures, subsequently increasing the resistance across the bulk region of the

solar cells. This reduces charge transportation towards the top and bottom electrodes. This also contributes to the decrease in the PCE and FF of the solar cells. Figure 7 plots the data from Table 4 directly: V_{oc} , FF, and PCE all decline steadily with increasing temperature from 280 to 400 K, while J_{sc} stays essentially flat, consistent with the mechanism described above. Additionally, MAPbI₃ undergoes a tetragonal-to-cubic phase transition at approximately 330 K, which lies within the investigated temperature range of 280–400 K. This transition may modify its bandgap, dielectric properties, carrier mobility, and recombination behavior. However, SCAPS-1D does not automatically account for structural phase transitions, and the materials' parameters were kept constant during the temperature sweep. Therefore, the results represent the electronic temperature-dependence of the device under the assumed material parameters, while possible phase transition effects constitute a limitation of the present model.

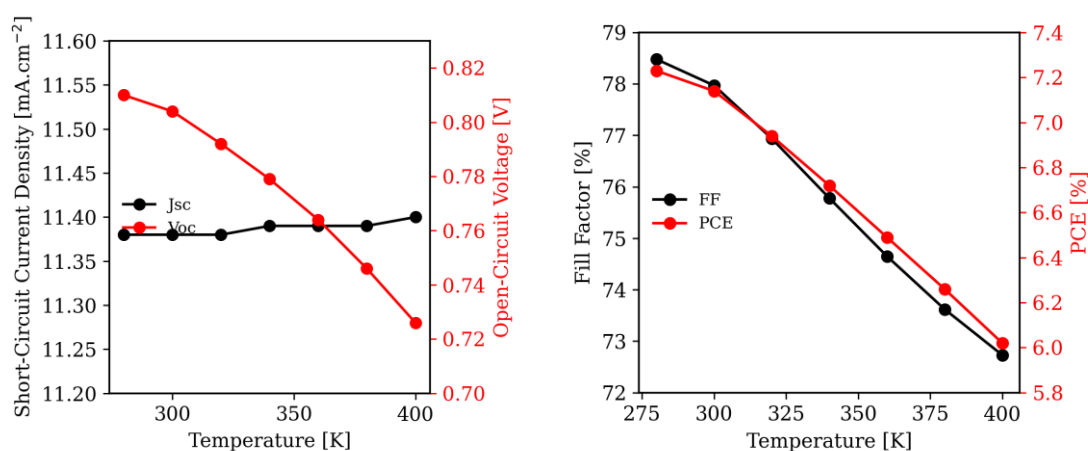


Figure 7. (a) J_{sc} and V_{oc} versus temperature. (b) FF and PCE versus temperature. Data correspond to Table 4.

Summary of single-parameter single-parameter versus combined optimization combined optimization

The preceding sensitivity sweeps (Figures 4–6) vary one MAPbI₃ parameter at a time while holding the others at their initial baseline values; none of these single-parameter sweeps alone reproduces the final device performance reported below. Table 5 summarizes this distinction before the combined optimization results are presented.

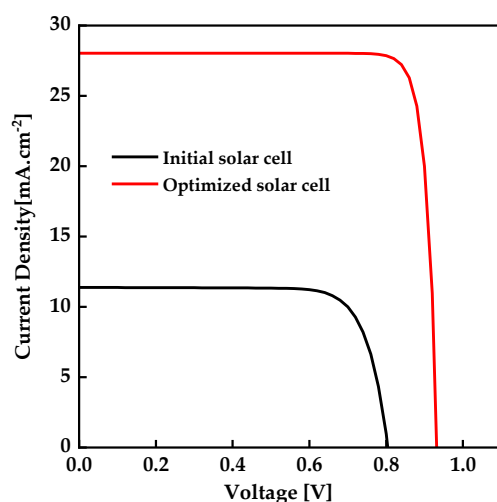
The final device outperforms either single-parameter optimum individually, indicating a synergistic effect between the absorber's thickness and doping density that is not captured by varying either parameter alone.

Table 5. Comparison of the baseline, single-parameter, and combined optimization results.

Stage	MAPbI ₃ thickness	Doping density	J_{sc} (mA/cm ²)	V_{oc} (V)	PCE (%) / FF (%)
Baseline (unoptimized)	0.1 μ m	1.0×10^{18} cm ⁻³	11.38	0.80	7.1/77.9
Thickness sweep only (Figure 4)	1.5 μ m	1.0×10^{18} cm ⁻³ (fixed)	25.97	0.835	16.7/76.9
Doping sweep only (Figure 5)	0.1 μ m (fixed)	1×10^{22} cm ⁻³	11.16	0.96	9.4/87.6
Final combined- optimized device (Figure 8)	1.2 μ m	1×10^{22} cm ⁻³	28.0	0.93	22.9/87.4

DC characteristics of optimized solar cells

Figure 8 shows the J–V characteristics of the optimized solar cells and compares them with those of nonoptimized solar cells. As can be seen, the optimization process led to a significant improvement in overall photovoltaic performance due to an increase in the J_{sc} and V_{oc} . For optimized solar cells, the J_{sc} is enhanced from 11.38 mA/cm² to 28.0 mA/cm², while the V_{oc} increases from 0.80 V to 0.93 V. The PCE significantly increased from 7.1% to 22.9%. This improvement is attributed to enhanced light harvesting because the optimized solar cell with an MAPbI₃ thickness of 1.2 μ m absorbs more incident photons, thereby generating a greater number of electron–hole pairs. On the other hand, the dopant density improves V_{oc} by strengthening the internal electric field and enhancing charge separation. It is thought that these increased electron–hole pairs contribute to the enhancement of the PCE.

**Figure 8.** Comparison of the current density–voltage (J–V) curves for the initial and optimized structures.

AC characteristics of the optimized solar cell

AC analysis is considered to be a powerful technique for probing the electronic properties, depletion region behavior, and defect density in PSCs [39]. Figure 9a shows the doping density–

dependent capacitance of our PSC device as the doping density of the MAPbI₃ is varied. At low bias voltages (<0.6 V), the capacitance remains nearly unaffected. In comparison, at higher bias values (>0.6 V), an apparent variation was observed, increasing rapidly to a maximum value in forward bias. The onset of the sudden increase and maximum capacitance density depended on the doping density. As the doping density increases, the rapid capacitance increase shifts toward higher voltages: The transition region shifts from approximately 0.44–0.56 V at a doping density of $1.0 \times 10^{18} \text{ cm}^{-3}$ to 0.68–0.80 V at $1.0 \times 10^{22} \text{ cm}^{-3}$.

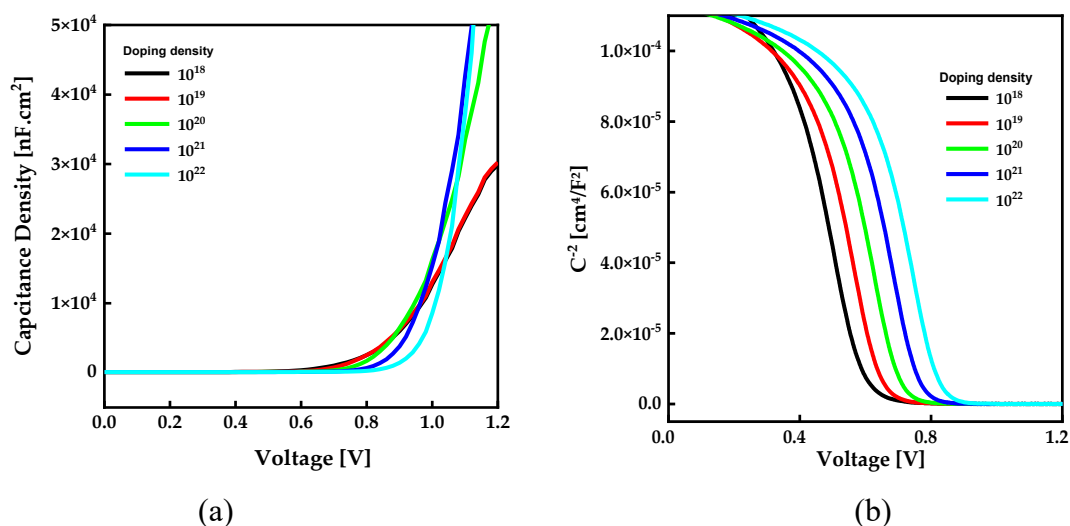


Figure 9. (a) Capacitance density vs voltage of the PSC device. (b) C^{-2} vs voltage of the PSC device.

The data in Figure 9a are replotted in Figure 9b as C^{-2} (inverse square of the capacitance) versus voltage, following standard Mott–Schottky analysis. The graph shows a linear region with steeper gradient in forward bias, revealing that the doping density strongly influences the electrical properties of the materials used in the device, thereby affecting the capacitance. This effect can be systematically analyzed using the Mott–Schottky approach. The intercept of the extended linear portion of the C^{-2} and voltage plots with the voltage axis produced $V_{bi} = 0.60 - 0.83$ V, approaching the V_{oc} of the device. The value of V_{bi} increased by increasing the doping density from $1.0 \times 10^{18} \text{ cm}^{-3}$ to $1.0 \times 10^{22} \text{ cm}^{-3}$. V_{bi} values of 0.60, 0.65, 0.71, 0.77, and 0.83 V were obtained for these five doping densities, respectively, rising steadily with doping and indicating reduced carrier recombination and series resistance. A higher V_{bi} reduces carrier recombination, lowers series resistance, and enhances the separation and collection of photogenerated carriers [40]. These improvements directly translate into a higher J_{sc} and FF, thereby boosting the overall PCE. Conversely, insufficient doping leads to a wider depletion region, weaker internal fields, and increased recombination, which reduces the V_{oc} and FF and ultimately the PCE.

Figure 10 shows the effect of the MAPbI₃ layer's thickness on the capacitance–voltage characteristics of the PSC. Like the previous results, at low bias voltages (<0.6 V), the capacitance density remains nearly unaffected, while it increases at higher bias values (>0.6 V). Interestingly, both the onset voltage of the rapid increase (~ 0.88 V) and the maximum capacitance density value were found to be independent of the MAPbI₃ layer's thickness, indicating that variation in the

thickness does not significantly influence this behavior. To further investigate this behavior, the data in Figure 10a are replotted in Figure 10b as C^{-2} vs voltage, following the standard Mott–Schottky analysis. The plots exhibit similar behavior to that observed for C^{-2} versus voltage, with a distinct linear region. This confirmed the presence of a well-defined space-charge region within the device. Additionally, from the extrapolation of the linear portion of the plot, the V_{bi} was determined to be approximately 0.80 V, which closely matches the V_{oc} of the solar cell. However, V_{bi} remained constant across different thicknesses of MAPbI₃, indicating that variation in the thickness does not affect the potential barrier at the interface. This result strongly suggests that the electrical properties of the PSC interface are primarily governed by the interfacial states and energy alignment, rather than the bulk thickness of the MAPbI₃.

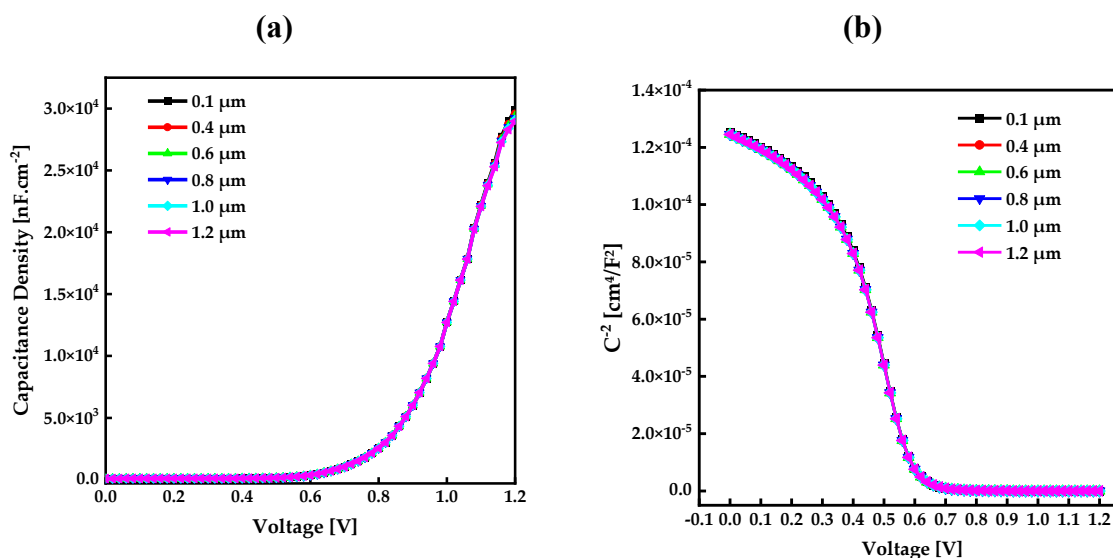


Figure 10. (a) Capacitance density vs voltage of the PSC. (b) C^{-2} vs voltage of the PSC.

However, the thickness of MAPbI₃ is essential for evaluating the efficiency and performance of PSCs' architecture. This was examined using Nyquist plots presenting the imaginary part Z_{Im} versus the real part Z_{Re} at different thicknesses of the perovskite layer (Figure 11). In this plot, the device with thinner layers exhibited larger semicircular arcs corresponding to higher resistance. As the thickness of the perovskite layer increases from 0.4 μm to 1.2 μm, the arc size decreases significantly. Under standard equivalent-circuit analysis of PSCs, the dominant midfrequency arc is assigned to recombination resistance (R_{rec}); a smaller arc therefore indicates a lower R_{rec} , i.e., increased recombination, rather than improved charge collection efficiency. This is consistent with the greater bulk recombination expected in thicker absorber layers [41].

The arc diameter is inversely related to the recombination rate: A larger arc corresponds to a higher recombination resistance and therefore more effective suppression of nonradiative losses, while a smaller arc indicates a lower recombination resistance and increased recombination. This trend highlights the importance of carefully tuning the perovskite layer's thickness to balance light absorption against the associated increase in bulk recombination at larger thicknesses.

The impedance response of PSCs provides information about charge transport, recombination, and dielectric processes occurring at distinct time scales. The Nyquist arcs (Figure 11) reflect the

competition between charge transfer and recombination, with the arc diameter being directly related to the recombination resistance. The reduction in arc diameter with increasing absorber thickness therefore indicates a decrease in recombination resistance, consistent with the greater volume available for SRH bulk recombination in thicker films. This does not contradict the increase in short-circuit current with thickness (Figure 4): Higher photocurrent stems from increased optical absorption, while the parallel decline in recombination resistance represents a competing loss mechanism that ultimately limits further gains in V_{oc} and FF at larger thicknesses. Mott–Schottky analysis (Figures 9b and 10b) provides the built-in potential through $(\frac{1}{C^2} = \frac{2(V_{bi}-V)}{q \epsilon \epsilon_0 N_A})$. The independence of V_{bi} from the absorber's thickness confirms that interfacial energetics, rather than bulk properties, dominate the electrostatics of this heterostructure.

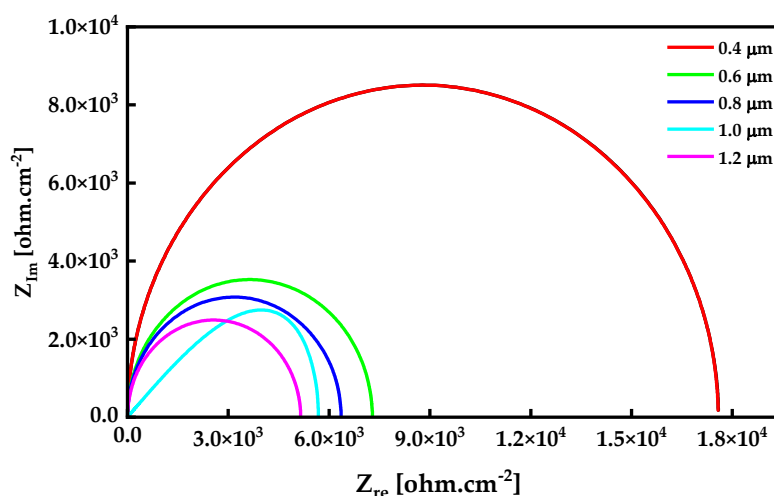


Figure 11. Impedance Nyquist plot showing the imaginary part versus the real part of impedance for different thicknesses of the MAPbI₃ absorber layer.

Comparison with the literature

To contextualize these results, Table 6 compares the present WO₃/MAPbI₃/GO device with two closely related SCAPS-1D studies from the same research group and one independent WO₃-based electron transport layer study. The TiO₂/MAPbI₃/GO device [17] uses an identical GO HTL and the same MAPbI₃ absorber but a different (TiO₂) ETL, isolating the effect of the choice of ETL. The ZnO–WO₃/CsPbIBr₂ device [14] uses the same WO₃-based ETL family but a different, all-inorganic absorber, isolating the effect of the absorber material.

Table 6. Comparison of the present WO₃/MAPbI₃/GO device with related SCAPS-1D studies.

Device (ETL/MAPbI ₃ L/HTL)	Baseline PCE	Optimized PCE	Optimized FF	Optimized Voc	Ref.
This work: WO ₃ /MAPbI ₃ /GO	7.1%	22.9%	87.4%	0.93 V	—
TiO ₂ /MAPbI ₃ /GO	11.6%	20.8%	80.5%	n.r.	[17]
ZnO–WO ₃ /CsPbIBr ₂	n.r.	12.87%	n.r.	n.r.	[14]

Note: n.r. = not reported in the cited abstract. The present device's optimized PCE (22.9%) exceeds both comparators, though the TiO₂/MAPbI₃/GO device [17] starts from a substantially higher unoptimized baseline (11.6% vs 7.1%), indicating a more favorable default band alignment with TiO₂ before optimization; the present WO₃-based device instead relies more heavily on the combined thickness–doping optimization to reach its final efficiency.

5. Conclusions

This study demonstrates the significant impact of optimizing the MAPbI₃ absorber layer's properties on the performance of WO₃/MAPbI₃/GO PSCs. Using SCAPS-1D simulations, systematic variation of the thickness, doping density, defect density, and electron affinity revealed clear optimization pathways. Increasing the absorber's thickness to 1.2 μm enhanced light absorption and photocurrent generation, though beyond this point, bulk recombination degraded performance. Optimizing the doping density to $1.0 \times 10^{22} \text{ cm}^{-3}$ strengthened the internal electric field, improving charge separation and raising V_{oc} from 0.80 V to 0.93 V. A defect density below 10^{14} cm^{-3} proved essential to minimize SRH recombination, while an electron affinity of 3.9 eV provided optimal conduction band alignment with the WO₃ transport layer. The combined optimization yielded a simulated power conversion efficiency of 22.9%, compared with 7.1% for the baseline structure. AC analysis through capacitance–voltage and impedance spectroscopy confirmed that optimized doping reduces series resistance and modifies the depletion region's behavior appropriately. These results provide guidance for experimental design of PSCs. However, the simulated efficiency represents a theoretical upper bound under idealized conditions. Practical devices with WO₃ and GO transport layers would likely achieve lower performance due to parasitic absorption, contact resistance, and interfacial recombination that cannot be fully captured in one-dimensional simulations.

Use of AI tools declaration

Artificial intelligence (AI)-assisted tools were used to support data verification, citation checking, and manuscript formatting during revision; all scientific content, interpretations, and conclusions were reviewed and approved by the authors.

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Author contributions

Hmoud Al Dmour: Conceptualization, methodology, software (SCAPS-1D simulation), validation, supervision, writing—original draft. Saleh R. Al-Bashaish: Formal analysis, investigation, data curation, Funding acquisition. Bonginkosi V. Kheswa: Validation, writing—review and editing. Selma Rabhi: Investigation, resources. Nabil Bouri: Software, visualization. Ahmad M. D. (Assa'd) Jaber: Formal analysis, resources. Ahmad Telfah: Validation, writing—review and editing. All authors have read and agreed to the published version of the manuscript.

Conflict of interest

All authors confirm that there are no conflicts of interest or personal relationships that might have seemed to affect the work presented in this article.

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