

Article

Design of MAPb(Br_xI_{1−x})₃-Based Solar Cells: Compositional Optimization for Thermally Stable and Defect-Tolerant Devices

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Abstract

Mixed halide perovskites can be tuned for bandgap, but they are prone to thermal defect deterioration that is difficult to evaluate throughout the whole stoichiometry range. Here, we investigate the relationship between Br composition, trap density, and temperature. It is observed that asymmetric thermal defect trade-offs provide predictive design principles beyond obvious efficiency trends. We use SCAPS-1D to model MAPb(Br_xI_{1−x})₃ solar cells. Simulation parameters include continuous bowing-corrected functions of Br fraction ($0 \leq x \leq 1$), temperature (300–350 K), and trap density (10^{11} – 10^{20} cm^{−3}). Despite a trade-off between short circuit current and open circuit voltage with Br incorporation (power conversion efficiency drops from ~25.5% at $x = 0$ to ~12% at $x = 1$), important results reveal non-trivial asymmetries: (i) Br-rich compositions are more sensitive to trap-assisted SRH recombination at $N_t > 10^{18}$ cm^{−3} than I-rich absorbers; (ii) the thermal degradation coefficient dV_{oc}/dT is lower for Br-rich systems than for I-rich systems, indicating improved thermal tolerance for Br-rich systems; and (iii) these quantitative design guidelines give predicted assistance for producing mixed halide perovskite devices with higher operational stability.

Keywords: solar cell; perovskite; MAPb(Br_xI_{1−x})₃; PEDOT:PSS; TiO₂; SCAPS-1D

1. Introduction

According to the recent NREL efficiency chart, lead-based perovskite solar cells have achieved more than 28% power conversion efficiency in single-junction configurations, thanks to extensive research efforts all around the world [1,2]. Now researchers are optimistic about the perovskite solar cell industry's future expansion [3,4]. But many researchers believe that lead-based toxicity will be the principal barrier to commercializing perovskite solar cells. However, lead-based toxicity can be minimized by using chemical additives, waterproof or self-healing encapsulation, partial lead replacement with suitable metals, halide mixing with bromide, or non-toxic metal substitution [5–15].

Compositional engineering of perovskite involves substituting lead ions in the crystalline structure of ABX₃ to minimize toxicity. Methylammonium lead iodide (MAPbI₃) is a very effective and well-researched perovskite material for compositional engineering [16]. However, the restricted tunability of the bandgap in MAPbI₃ limits the possibilities for improving optical properties compared to halide mixing. Generally, the perovskite absorber



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MAPbI₃ is sensitive to degradation and phase transition at high temperature, as well as after water molecule adsorption [17]. This inherent instability is a significant challenge for long-term device operation and needs to be tackled through stable perovskite compositions or encapsulation strategies for practical viability.

The energy bandgap of MAPb(Br_xI_{1-x})₃ may be controlled from 1.55 eV to around 2.3 eV by altering the bromide content (x), making it promising for efficient solar cells. Compositional engineering of MAPb(Br_xI_{1-x})₃ alters the structural, electrical, mechanical strain, optical, and thermal characteristics as the Br level increases. The optimal Br concentration for overcoming the inherent instability of MAPb(Br_xI_{1-x})₃ through compositional engineering is a highly discussed issue in recent literature [18–20].

Many previous numerical studies neglected to account for the important interaction that occurs when these parameters, such as compositional tuning, thermal effects, and defect density, are changed simultaneously. The purpose of this study is to address this gap by modeling the compositional tuning, thermal effects, and defect density (x, T, and N_t) dependence of Voc, Jsc, FF, and PCE. It then parameterizes all significant photovoltaic properties as continuous, bowing-corrected functions of Br fraction x across the whole compositional range (0 ≤ x ≤ 1). This work investigates the temperature-dependent electrical performance of MAPb(Br_xI_{1-x})₃-based devices. These insights may help create compositions with lower thermal sensitivity. However, thorough stability evaluation requires further experimental confirmation of the real degradation processes [20–25].

The toxicity and stability of MAPb(Br_xI_{1-x})₃ perovskite may be influenced by the relative concentration of Br and I because of structural and chemical changes in mixed halide systems. Numerous experimental studies have shown that the incorporation of Br can improve the stability of the material with respect to moisture and phase transitions [17–19], but the overall toxicity is less clear (partial replacement of Br reduces the iodine content, but lead is the main toxic species). This numerical study complements this understanding by quantifying the role of Br concentration (x) in tuning the defect tolerance and thermal resilience and helps to identify compositions that can not only balance efficiency and stability, but also reduce the dependence on toxic lead through compositional optimization.

In this study, a comprehensive numerical analysis of absorber MAPb(Br_xI_{1-x})₃-based perovskite solar cells is carried out for the whole absorber compositional (0 ≤ x ≤ 1) range, with TiO₂ as the electron transport layer (ETL) and PEDOT:PSS as the hole transport layer (HTL). The parameters for all important optoelectronic material characteristics, including bandgap, electron affinity, carrier mobility, and dielectric permittivity, are defined as continuous functions of Br percent x that account for bending correction, according to previous experimental evidence. To fully evaluate the contributions of recombination across all compositions, the operating temperature is systematically changed from 300 to 350 K, and the trap density is swept from 10¹¹ to 10²⁰ cm⁻³. The following variables are taken into consideration and examined as interdependent functions of halide composition x, temperature T, and trap density N_t: open circuit voltage (V_{oc}), short circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE). In order to create thermally stable and defect-tolerant MAPb(Br_xI_{1-x})₃ perovskite photovoltaic devices that can withstand real-world operating conditions, the results that were obtained reveal composition-dependent asymmetries in thermal resilience and sensitivity between Br-rich and I-rich compositions.

The energy bandgap and electron affinity of perovskite materials are critically determined by the ratio of Br and I concentration. Substitution of iodide by bromide leads to an increased bandgap by a downshift of the valence band maximum. This is mainly caused by halide p-orbital contributions [26]. Such tunability has a direct impact on the ionization potential and electron affinity that characterize the absolute energy levels. The device performance is strongly dependent on the optimal band alignment at the interfaces

of the perovskite/charge transport layers. Conduction band offsets of 0.0–0.3 eV and appropriately positioned valence bands minimize recombination and permit efficient charge collection. This is borne out by theoretical analysis [27]. This results in a “cascade” band alignment that facilitates smooth charge transport, as opposed to detrimental “cliff” or “spike” alignments [28]. So, halide composition engineering is a powerful tool for both tuning the bandgap and optimizing the energy landscape of the whole device.

To the best of authors’ knowledge, the combined interdependencies of bromide composition, trap density, and operating temperature on the photovoltaic performance of MAPb(Br_xI_{1−x})₃ perovskite solar cells have not been investigated before. While a number of SCAPS-1D-based studies have been performed to explore compositional engineering, defect density, and temperature effects in perovskite systems [20–25], these factors have often been examined in isolation or over a limited compositional range. For example, mixed halide MAPb(I_{1−x}Cl_x)₃ devices were improved by Paz Totolhua et al. by tuning thickness, defect density, and contact work function [29]. Some studies have been conducted on MAPbI₃ performance as a function of temperature or effects of chloride inclusion [30,31]. However, none of these studies consider the interdependence of full-range halide composition ($x = 0$ to 1), wide-range trap density (10^{11} – 10^{20} cm^{−3}), and operating temperature (300–350 K) in a single framework. This work aims to fill the gap by simulating the compositional tuning, thermal effects, and defect density dependency of open circuit voltage, short circuit current, fill factor, and power conversion efficiency throughout the entire compositional range. All the key optoelectronic material parameters, such as the bandgap, electron affinity, carrier mobility, and dielectric permittivity, are parameterized as continuous bowing-corrected functions of Br percent x , based on experimental data. The comprehensive coupled study exposes the composition-dependent asymmetry of heat resilience and trap sensitivity between Br-rich and I-rich compositions, which was absent in single-variable experiments. This work offers insights into the temperature dependent electrical performance of MAPb(Br_xI_{1−x})₃-based devices and may guide the development of lower thermally sensitive compositions. However, detailed stability assessment requires additional experimental confirmation of degradation pathways.

2. Simulation Methods and Device Structure

2.1. SCAPS-1D Simulation Framework

SCAPS-1D was selected for this study because SCAPS-1D (i) is a physics-based simulator for multilayer thin-film devices; (ii) solves carrier transport and recombination (e.g., SRH, radiative, and Auger); (iii) supports defect and interface modeling; (iv) predicts key performance metrics used in studies; (v) provides carrier/recombination profiles and band diagrams; (vi) enables sensitivity studies and identification of dominant loss mechanisms; (vii) supports realistic stack representation (thickness, doping, and mobilities) with boundary/contact conditions; (viii) allows calibration to experimental data; and (ix) enables fast, cost-effective optimization and literature-comparable modeling assumptions [32–35].

2.2. Mathematical Models Employed for Simulation

The complete mathematical formulations of the semiconductor transport and recombination models employed in this study, along with the full list of investigated device compositions, are provided in the Supplementary Materials (Equations (S1)–(S15) and Table S1) [36–48].

To facilitate a clear comparison, the electron transport layer and hole transport layer are standardized across all eleven devices, using titanium dioxide (TiO₂) for the electron transport layer and poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) PEDOT:PSS for the hole transport layer. All eleven devices use the standard n-i-p planar heterojunction

architecture: FTO/TiO₂/MAPb(Br_xI_{1-x})₃/PEDOT:PSS/Au, as shown in Figure 1. The essential optoelectronic material characteristics such as bandgap, electron affinity, carrier mobility, and dielectric permittivity are expressed as continuous, bowing-corrected functions of the Br fraction x , grounded in proven experimental data. The operating temperature ranges from 300 K to 350 K, and the trap density varies from 10¹¹ to 10²⁰ cm³ to comprehensively assess the contributions of Shockley–Read–Hall recombination across all compositions [49,50].

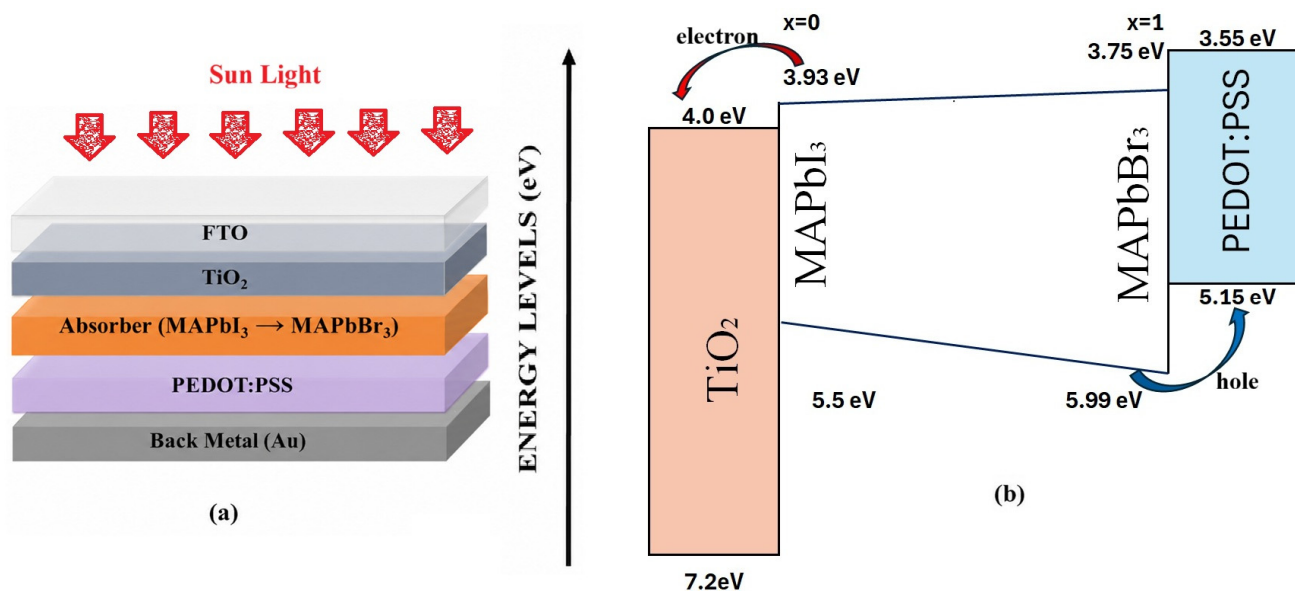


Figure 1. (a) Cross-section architecture of the perovskite solar cell (FTO/TiO₂/MAPb(I_{1-x}Br_x)₃/PEDOT:PSS/Au). (b) Corresponding energy level diagram showing electron and hole transport pathways.

2.3. Simulation Material Parameters

All material properties used in the SCAPS-1D simulations are derived from well-accepted experimental and theoretical literature to guarantee physical correctness and repeatability [49–64]. The data for the fixed transport layers, namely the TiO₂ electron transport layer (ETL) and PEDOT:PSS hole transport layer (HTL), including bandgap, electron affinity, carrier mobility, effective density of states, and doping concentrations, are sourced directly from extensively referenced SCAPS-1D perovskite simulation studies. For the MAPb(Br_xI_{1-x})₃ absorber layer, all essential optoelectronic characteristics are characterized as linear, composition-dependent functions of the bromide fraction x through Vegard's law with an optical bowing correction, which is commonly described as Equation (1) [55,56].

$$P(x) = P_I (1 - x) + P_{Br}(x) - b_p(1 - x) \quad (1)$$

Here, $P(x)$ denotes a composition-dependent material property, with P_I and P_{Br} representing the values of the pure iodide (MAPbI₃) and pure bromide (MAPbBr₃) end members, respectively. The parameter b_p is specific to each property. The bandgap and electron affinity are calculated using experimentally validated bowing parameters of $b_{Eg} = 0.33$ eV and $b_\chi = 0.06$ V, respectively, while the relative dielectric permittivity ϵ_r and carrier mobilities μ_n and μ_p are linearly interpolated between the end member values. For optical modeling, the SCAPS-1D software has several algorithms that may support multiple designs for forecasting the absorption coefficient [49,56,60–64].

Similarly, the given Equation (2) is a commonly used computational approach for evaluating the optical absorption coefficient model for any type of solar cell, including

perovskite solar cells (PSCs), where A and B are constants, h is a Planck constant, ν represents the photon frequency, and E_g is the energy bandgap of the absorber material [40]:

$$\alpha = A + \frac{A}{h\nu} \sqrt{h\nu - E_g} \quad (2)$$

Tables 1 and 2 summarize all the input-required physical and material parameters that were used in the proposed simulation study.

Table 1. SCAPS-1D simulation parameters for TiO_2 (electron transport layer), PEDOT:PSS (hole transport layer), and $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ absorber layer for all eleven devices (D1–D11).

Parameter	Unit	TiO_2 (ETL)	PEDOT:PSS (HTL)	$\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$
Thickness	nm	50	50	500
Energy bandgap, E_g	eV	3.20	1.60	see Table 2
Electron affinity, χ	eV	4.00	3.55	see Table 2
Relative permittivity, ϵ_r	—	9.0	3.0	see Table 2
CB effective DOS, N_C	cm^{-3}	2.0×10^{18}	2.2×10^{18}	2.5×10^{18}
VB effective DOS, N_V	cm^{-3}	1.8×10^{19}	1.8×10^{19}	2.5×10^{18}
Electron mobility, μ_n	$\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$	20	1.0×10^{-4}	see Table 2
Hole mobility, μ_p	$\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$	10	1.0×10^{-4}	see Table 2
Electron thermal velocity, $v_{th,n}$	cm s^{-1}	1.0×10^7	1.0×10^7	1.0×10^7
Hole thermal velocity, $v_{th,p}$	cm s^{-1}	1.0×10^7	1.0×10^7	1.0×10^7
Doping concentrations				
Donor concentration, N_D	cm^{-3}	1.0×10^{18}	0	0
Acceptor concentration, N_A	cm^{-3}	0	1.0×10^{18}	0
Defect (trap) parameters				
Defect density, N_t	cm^{-3}	1.0×10^{15}	1.0×10^{15}	10^{11} – 10^{20} (swept)
Trap energy level, E_t	eV	Mid-gap	Mid-gap	Mid-gap
Capture cross-section (e^-), σ_n	cm^2	1.0×10^{-15}	1.0×10^{-15}	1.1×10^{-15}
Capture cross-section (h^+), σ_p	cm^2	1.0×10^{-15}	1.0×10^{-15}	1.1×10^{-15}
Recombination parameters				
Radiative recombination coefficient, B	$\text{cm}^3 \text{s}^{-1}$	0	0	2.3×10^{-9}
Auger coefficient, α	$\text{cm}^3 \text{s}^{-1}$	0	0	1.0×10^{-29}
Absorption model (Tauc law)				
Absorption constant, A	$\text{cm}^{-1} \text{eV}^{-1/2}$	1.0×10^4	1.0×10^4	1.0×10^3
Contact parameters				
Front contact work function (FTO)	eV	4.40	-	-
Back contact work function (Au)	eV	5.10	-	-
Front surface recombination velocity, v_{th}	cm s^{-1}	1.0×10^7	-	-
Back surface recombination velocity, v_{th}	cm s^{-1}	1.0×10^7	-	-
References		[65–67]	[68–71]	[49–64]

Table 2. Material properties of the perovskite absorber layer (MAPb(Br_xI_{1−x})₃) as a function of composition derived from Equation (16) for devices D1–D11.

Device	x	Absorber	E _g (eV)	χ (eV)	ε _r	μ _n = μ _p (cm ² V ^{−1} s ^{−1})
D1	0.0	MAPbI ₃	1.570	3.930	25.5	22.0
D2	0.1	MAPb(Br _{0.1} I _{0.9}) ₃	1.607	3.912	25.0	21.2
D3	0.2	MAPb(Br _{0.2} I _{0.8}) ₃	1.651	3.894	24.4	20.3
D4	0.3	MAPb(Br _{0.3} I _{0.7}) ₃	1.703	3.875	23.8	19.5
D5	0.4	MAPb(Br _{0.4} I _{0.6}) ₃	1.761	3.856	23.1	18.6
D6	0.5	MAPb(Br _{0.5} I _{0.5}) ₃	1.824	3.836	22.4	17.7
D7	0.6	MAPb(Br _{0.6} I _{0.4}) ₃	1.892	3.815	21.7	16.7
D8	0.7	MAPb(Br _{0.7} I _{0.3}) ₃	1.962	3.794	20.9	15.7
D9	0.8	MAPb(Br _{0.8} I _{0.2}) ₃	2.034	3.773	20.1	14.6
D10	0.9	MAPb(Br _{0.9} I _{0.1}) ₃	2.106	3.751	19.3	13.5
D11	1.0	MAPbBr ₃	2.240	3.750	17.0	10.0

2.4. Simulation Framework

Firstly, both transport layers, TiO₂ and PEDOT:PSS, are optimized in terms of thickness and doping density as a precondition for research, and then the MAPb(Br_xI_{1−x})₃ layer thickness is varied from 100 nm to 1000 nm in uniform increments to identify the optimal thickness that maximizes power conversion efficiency for each device. The bulk trap density N_t is independently swept from 10¹¹ cm^{−3} to 10²⁰ cm^{−3} at mid-gap energy to quantify Shockley–Read–Hall recombination contributions as a function of halide composition x.

Operating temperature is systematically varied from 300 K to 350 K in steps of 10 K to evaluate thermally activated carrier transport, ion migration, and recombination rate enhancement across all compositions. Additional recombination parameters investigated include the carrier lifetimes and diffusion coefficient. The extracted photovoltaic output parameters, open circuit voltage, short circuit current, fill factor, and power conversion efficiency are analyzed as coupled functions of all swept variables to construct a complete performance landscape for each of the eleven absorber compositions. The step-by-step simulation procedure used in this study is illustrated in Figure 2.

The device architecture used in this work is FTO/TiO₂/Perovskite/PEDOT:PSS/Au, which is a regular n-i-p architecture with TiO₂ as the electron transport layer and PEDOT:PSS as the hole transport layer. PEDOT:PSS is mostly used in inverted (p-i-n) configurations, but its application in normal n-i-p architectures has been experimentally demonstrated by different processing methods such as water-free PEDOT:PSS dispersions [72], WO₃/PEDOT:PSS composites (15.1% efficiency) [73], solvent-free transfer lamination [74], ALD-assisted interfacial engineering (11% efficiency) [75], toluene-dispersed PEDOT ink (14.5% efficiency) [76], alcohol-dispersed PEDOT:F complexes (24.5% efficiency) [77], transfer printing [78], and dopant-free spiro-OMeTAD/PEDOT mixtures (18.7% efficiency) [79].

The key requirement for any hole transport layer in an n-i-p configuration is energy level alignment with the perovskite valence band, and photoelectron spectroscopy has confirmed the type II band alignment of the heterojunction, enabling efficient hole extraction and electron blocking [49–53]. Importantly, our central objective—investigating the coupled effects of bromide composition, trap density, and temperature on recombination dynamics and performance—is architecture-independent, as the physical principles gov-

erning defect tolerance, thermal resilience, and composition-dependent asymmetries are fundamental material properties applicable to both n-i-p and p-i-n configurations. All simulation parameters are derived from experimentally validated material properties.

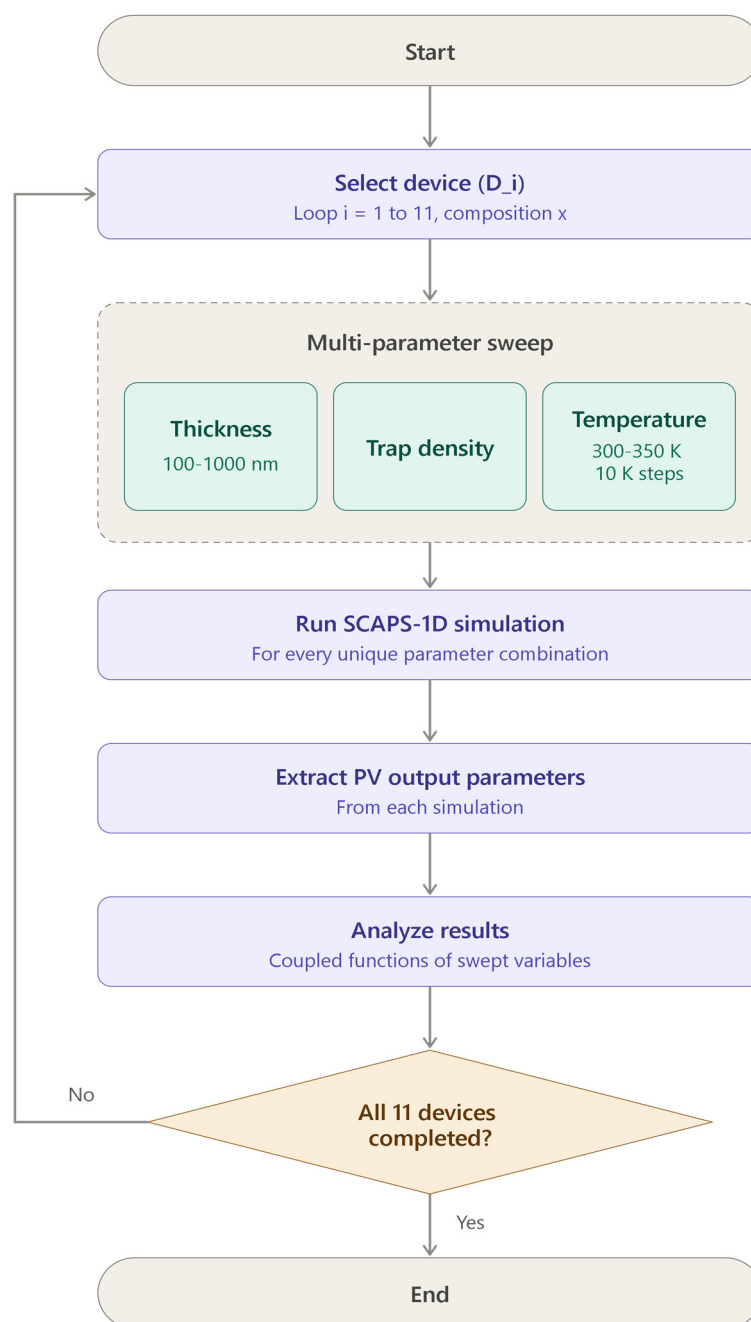


Figure 2. Systematic simulation flowchart for the proposed photovoltaic devices based on perovskite absorber $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ for D1 to D11 devices.

3. Results

3.1. Photocurrent–Voltage Responses of the Proposed Devices

Photocurrent–voltage characterization is one of the most important techniques for analyzing the overall behavior of the basic photovoltaic solar cell. Figure 3 depicts the overall photovoltaic response as current–voltage (J–V) characteristics of $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ perovskite solar cells throughout the whole compositional range, from $x = 0$ to 1. All devices exhibit the typical photovoltaic behavior of solar cells. Where a smooth photocurrent

plateau is formed at low forward bias, it is followed by a sharp decline approaching the open circuit voltage, signifying efficient carrier collection under short circuit conditions and diode-dominated recombination near the open circuit voltage. A consistent trade-off is observable in the compositions, as the increasing bromide content (x) progressively reduces the short circuit current density, consistent with the widening optical bandgap that blue-shifts the absorption onset and narrows the spectral collection range. Simultaneously, the J–V curve advances to higher voltages as x increases, indicating an enhanced open circuit voltage due to the increased quasi-Fermi level splitting in wider-gap absorbers. The interplay between the declining photocurrent and the rising voltage output dictates the overall power conversion efficiency of any composition [80,81].

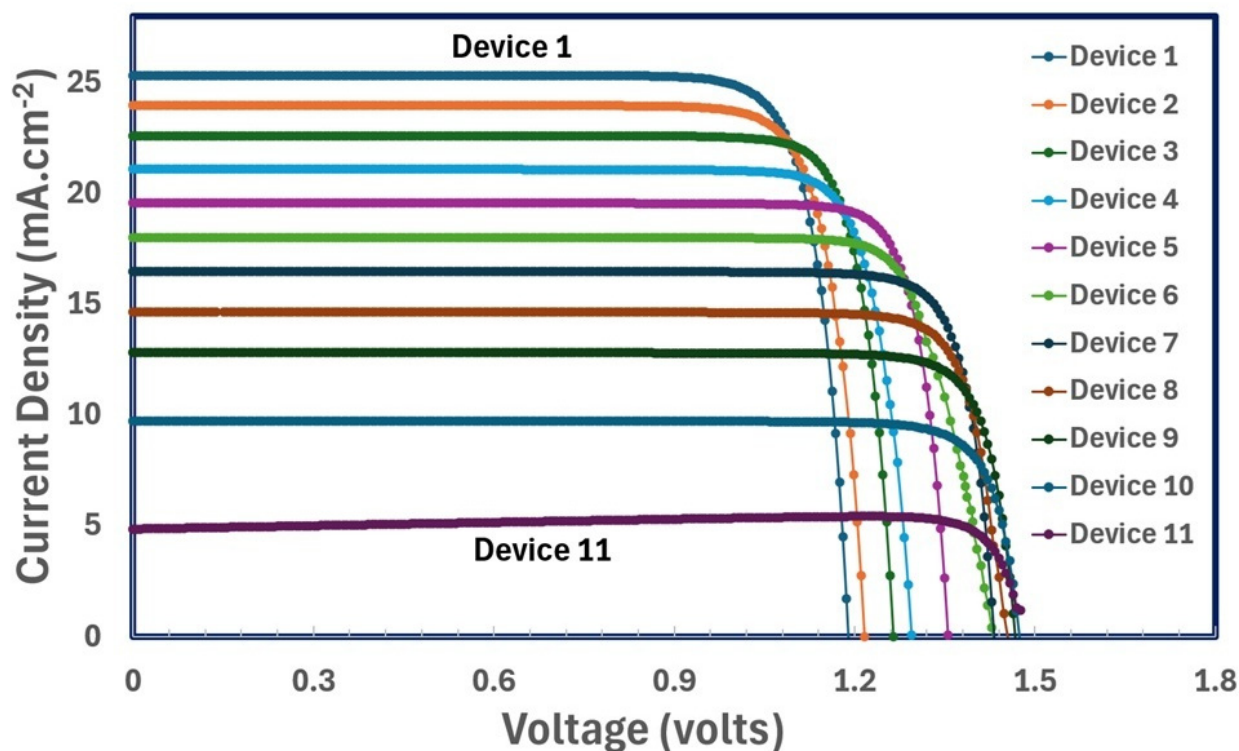


Figure 3. Current density–voltage (J – V) characteristics of $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ -based perovskite solar cells for devices D1–D11 with varying bromide fraction ($x = 0.0$ – 1.0).

3.2. Effects of Bromide Concentration on Photovoltaic Performance Parameters

Figure 4 illustrates the photovoltaic performance parameters, such as (a) open circuit voltage, (b) short circuit current, (c) fill factor, and (d) power conversion efficiency of $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ -based devices (D1–D11). The figure clearly demonstrates that all devices exhibit a clear dependence on the bromide fraction x , which increases from 0 to 1.0. As the Br content (x) of $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ increases, the open circuit voltage (see Figure 4a) shows a steady enhancement from ~ 1.18 V (D1, $x = 0.0$) to ~ 1.5 V (D11, $x = 1.0$). This improvement is attributed, maybe, to the widening of the perovskite bandgap with increasing bromide incorporation [59]. Conversely, the short circuit current density (see Figure 4b) decreases monotonically from $\sim 24.5 \text{ mA}\cdot\text{cm}^{-2}$ to $\sim 9.5 \text{ mA}\cdot\text{cm}^{-2}$ over the same compositional range as x , reflecting reduced photon absorption due to the broader bandgap. The fill factor (see Figure 4c) also shows a small but steady improvement, going from about $\sim 83.8\%$ at $x = 0$ to about $\sim 86.9\%$ at almost $x = 0.7$ and then going down to about $\sim 86.3\%$ at $x = 1$. This means that more charge is being extracted and less charge is being lost through recombination at higher bromide fractions. However, the power conversion efficiency shows a decreasing trend (see Figure 4d). The power conversion efficiency declines from

~25.5% at $x = 0.0$ (MAPbI₃) to ~12% at $x = 1$ (MAPbBr₃), mainly due to the significant reduction in photocurrent despite the gains in open circuit voltage and fill factor, as shown in Figure 4a,c. These results clearly demonstrate that intermediate compositions of the Br fraction (x) cause a decrease in the power conversion efficiency performance of photovoltaic devices [60].

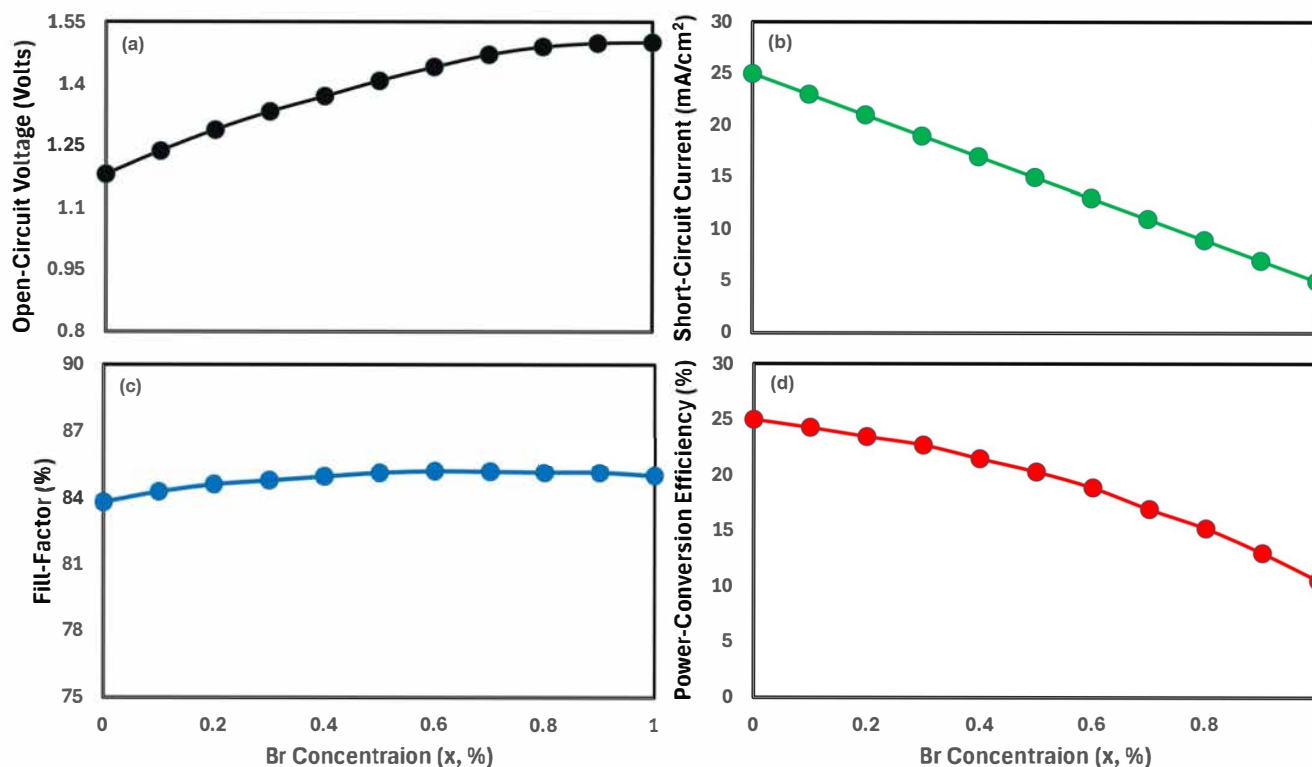


Figure 4. Photovoltaic performance parameters of MAPb(Br _{x} I_{1- x})₃-based devices (D1–D11) as a function of bromide fraction (x). (a) Open circuit voltage, (b) short circuit current density, (c) fill factor, and (d) power conversion efficiency.

3.3. Effects of Bromide Concentration on External Quantum Efficiency

Photocurrent–voltage characterization does not convey the complete performance picture of the proposed photovoltaic devices. Therefore, external quantum efficiency analysis is performed for correlating the compositionally dependent optical absorption with the electrical output, as present in Figure 5. The external quantum efficiency spectra for selected devices ($x = 0.0$ (MAPbI₃), 0.2, 0.4, 0.6, 0.8, and 1.0 (MAPbBr₃)) exhibit a gradual blue shift in the absorption onset with increasing bromide content, which is consistent with the widening of the bandgap [82]. It is further observed that all devices effectively collect free charge carriers at their respective electrodes with negligible recombination losses, since the external quantum efficiency is more than 80% throughout a broad range of wavelengths [83]. The intermediate composition range between $x = 0$ and $x = 1$ has a slightly better external quantum efficiency response in comparison to longer wavelengths. Such improvement might be due to better film quality or decreased fault density. Overall, the integrated EQE spectra yield short circuit current values that are in excellent agreement with those derived from the photocurrent–voltage characteristics, thereby confirming the reliability of the measured photocurrents across all devices.

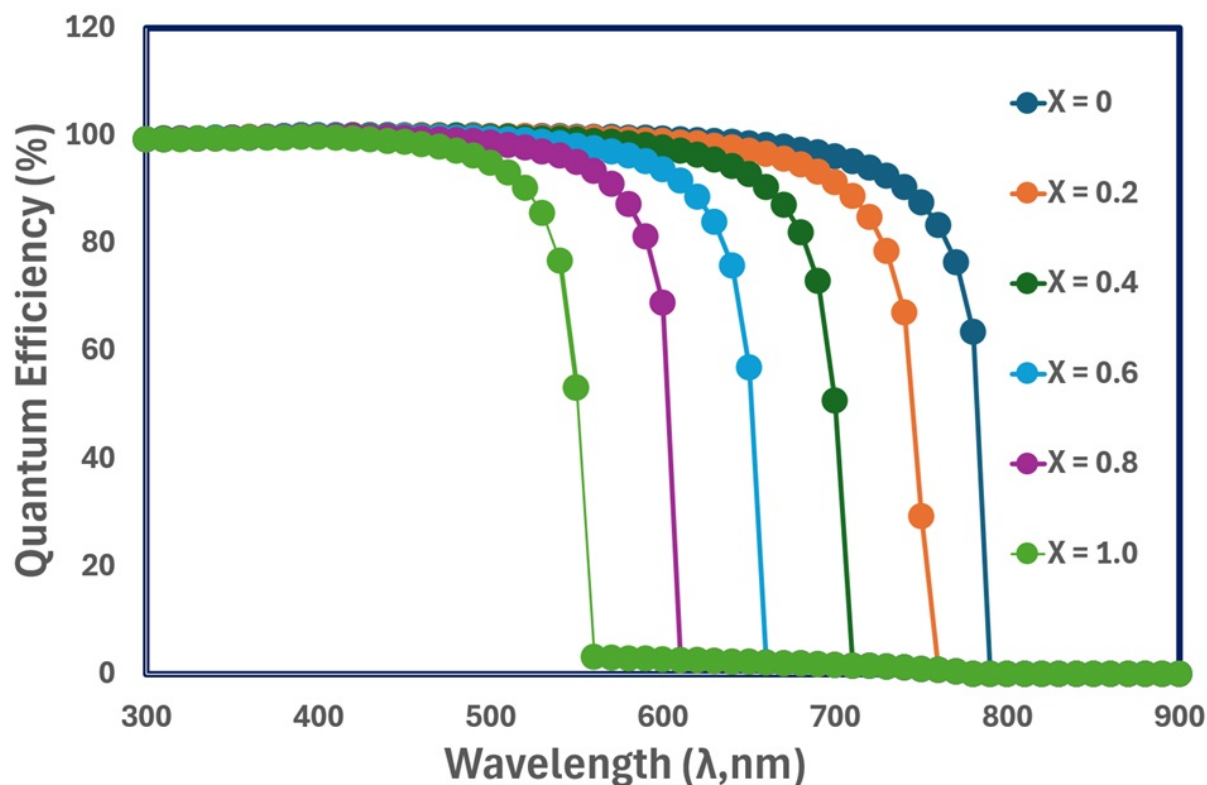


Figure 5. External quantum efficiency (EQE) spectra of the selected MAPb(Br_xI_{1-x})₃ devices ($x = 0.0, 0.2, 0.4, 0.6, 0.8$, and 1.0) as a function of wavelength.

3.4. Effects of Trap Density on Photovoltaic Performance Parameters

Trap density analysis is crucial for measuring photovoltaic devices performance, because it helps understand the defects' behavior that causes the electron–hole recombination process. The efficient control of the recombination process in terms of defect density plays a vital role in minimizing energy loss and maximizing the cell's power conversion efficiency [84,85]. Therefore, in order to investigate bulk defects affecting device performance, the trap density (N_t) in the absorber layer MAPb(Br_xI_{1-x})₃ was systematically changed for certain compositions of Br ($x = 0.0, 0.2, 0.4, 0.6, 0.8$, and 1.0) from 10^{11} to 10^{20} cm⁻³, as illustrated in Figure 6a–d. The figures clearly established that all compositions exhibit very similar trends for (a) open circuit voltage, (b) short circuit current density, (c) fill factor (FF), and (d) power conversion efficiency across the whole trap density range. At the highest defect density ($N_t > 10^{18}$ cm⁻³), photovoltaic parameters, especially power conversion efficiency, show slight variations for each device.

To further elaborate on the impact of Br contents (x) on photovoltaic device performance, the photovoltaic parameters were simulated across a range of Br contents (x) at three defect levels in Figure 7. As shown in the figure, the (a) open circuit voltage, (b) short circuit current density, and (c) fill factor remain largely stable at low-to-moderate trap densities (from 10^{11} up to 10^{14} cm⁻³), which indicates that the devices exhibit reasonable tolerance to bulk recombination centers [86]. However, at higher trap densities (10^{18} – 10^{19} cm⁻³), a pronounced degradation in all performance metrics is observed, which may be attributed to enhanced Shockley–Read–Hall recombination that reduces the carrier extraction efficiency [87]. The decay amount seems to change with the bromide level, which may mean that the Br composition affects defect tolerance. High trap density generates a large density of electronic energy levels inside the forbidden bandgap. Photogenerated electrons and holes quickly fill these trap states instead of remaining free in the conduction and valence bands. This immobilizes the charges and “pins” the quasi-Fermi levels to the

trap energy levels [88], which in turn causes the devices to exhibit almost identical power conversion efficiency (PCE) as a function of Br concentration (x), as observed in Figure 7.

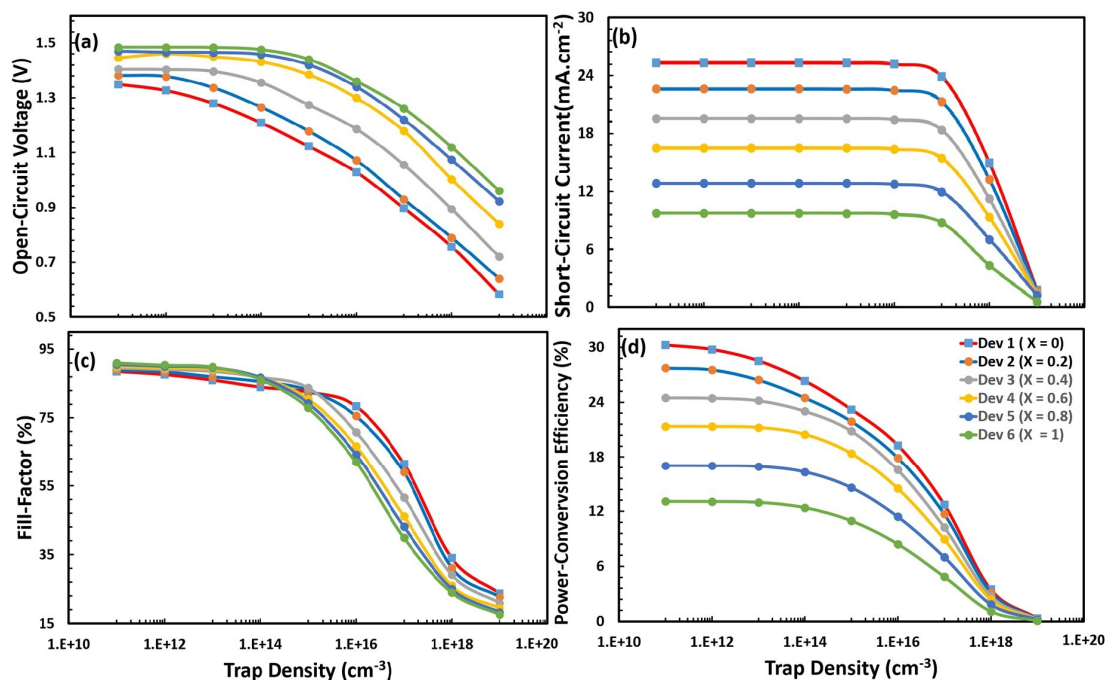


Figure 6. Photovoltaic parameters. (a) Open circuit voltage, (b) short circuit current, (c) fill factor, and (d) power conversion efficiency of MAPb(Br_xI_{1-x})₃ devices ($x = 0.0, 0.2, 0.4, 0.6, 0.8$, and 1.0) as a function of bulk trap density (N_t).

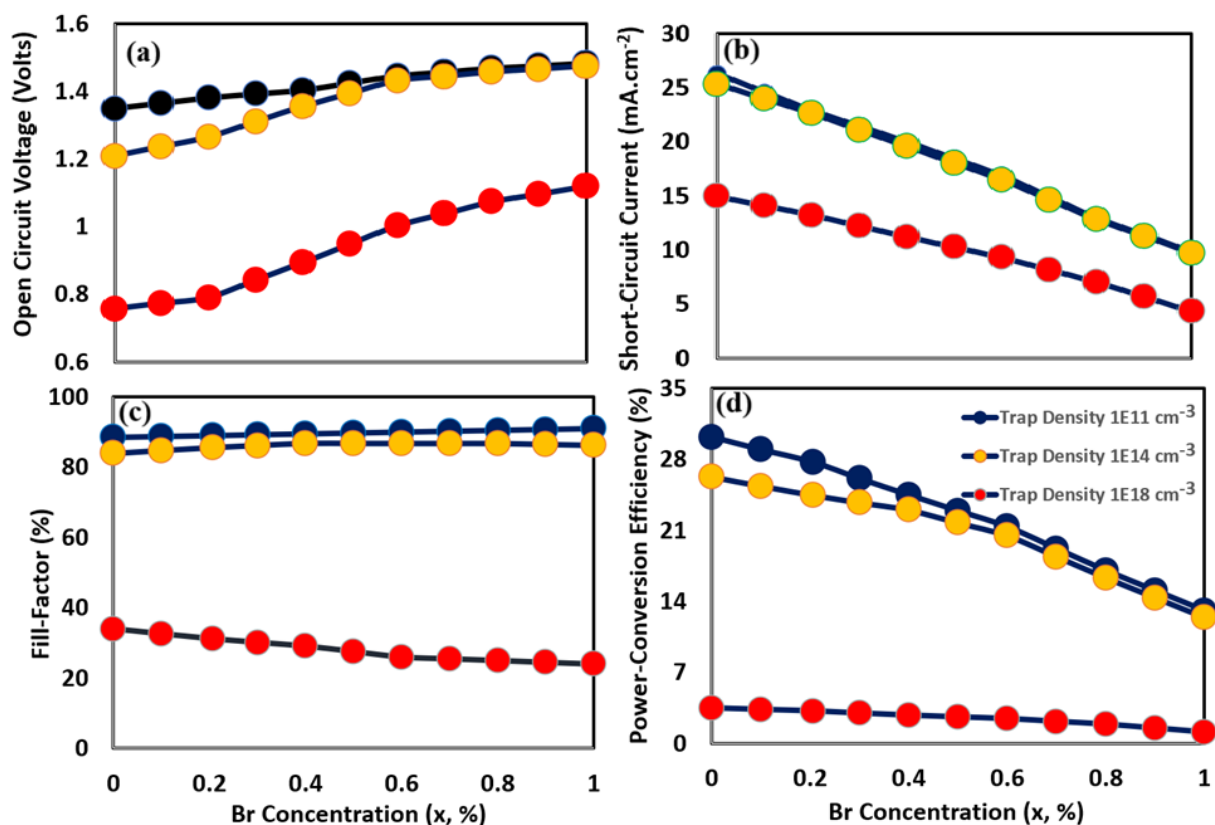


Figure 7. Photovoltaic parameters. (a) Open circuit voltage, (b) short circuit current, (c) fill factor, and (d) power conversion efficiency of MAPb(Br_xI_{1-x})₃ devices as a function of Br concentration (x) at three levels of bulk trap density (N_t): 10^{11} , 10^{14} , and 10^{18} cm⁻³.

3.5. Effects of Trap Density on Saturation Current

Saturation current density (J_0) is another important parameter used to measure the performance of perovskite solar cells. Saturation current density controls the open circuit voltage and qualitatively reflects the internal recombination losses. Therefore, reducing the saturation current density as much as possible is the main objective for efficient photovoltaic design. The mathematical relation between open circuit voltage and saturation current density can be defined as Equation (3) [37,38]:

$$V_{OC} = \frac{nkT}{q} \ln \left(\frac{J_{SC}}{J_0} + 1 \right) \quad (3)$$

where n is the diode ideality factor. The diode ideality factor indicates the extent to which the solar cell's current–voltage characteristics deviate from the ideal diode's equation. In most cases, the diode ideality factor is very close to 1.5 for many perovskite solar cells [89]. As in Figure 6, we have already determined the short circuit current and open circuit voltage for trap densities from 10^{11} to 10^{20} . Therefore, J_0 is calculated as a function of trap density from Equation (4), and the output response is displayed in Figure 8 [37,38].

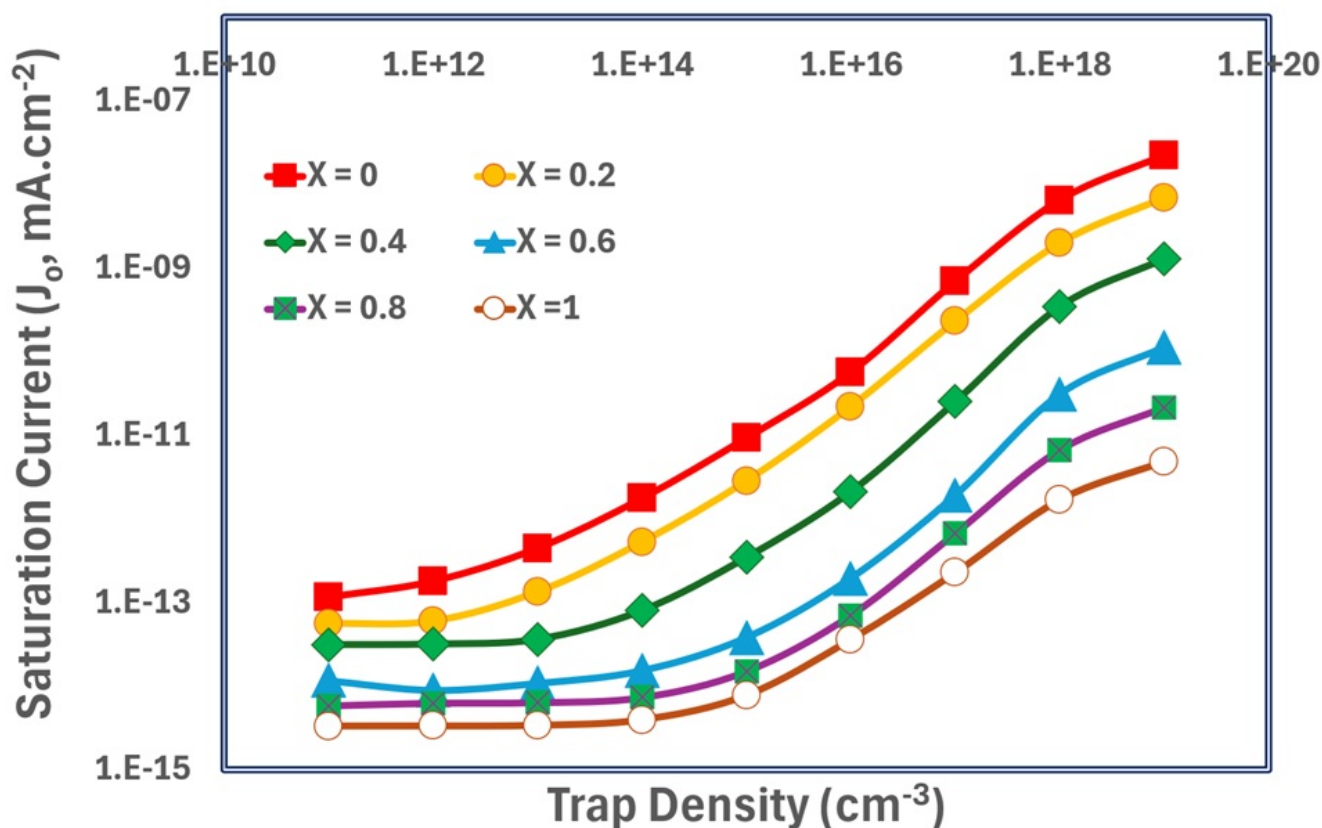


Figure 8. Saturation current density (J_0) of the selected MAPb(Br_xI_{1-x})₃-based perovskite photovoltaic devices ($x = 0.0, 0.2, 0.4, 0.6, 0.8$, and 1.0) as a function of trap density.

$$J_0 = \frac{J_{sc}}{\exp\left(\frac{qV_{oc}}{nkT}\right) - 1} \quad (4)$$

The impact of bulk defects in the absorber layer, MAPb(Br_xI_{1-x})₃, on charge carrier dynamics was investigated by plotting the saturation current density (J_0) against trap density (N_t) over the compositional concentration of Br in terms of x . All bromide fractions show a monotonic rise in J_0 with increased N_t , as shown in Figure 8. This agrees with the estimated increment in dark current mediated by Shockley–Read–Hall recombination [90].

At all trap densities, the saturation current is rather constant regardless of the halide content, indicating that the recombination kinetics are controlled more by the concentration of defects than by mobility or bandgap fluctuations in mixed halide systems [91,92], as observed for many other devices.

3.6. Effects of Br Concentration on Carrier Lifetime

Free electron and hole pairs are generated inside the perovskite absorber layer in response to light striking a perovskite solar cell. These pairs have a high probability of recombination after traveling a certain distance inside the absorption layer. Therefore, carrier lifetime is defined as the average amount of time an electron and a hole remain as free carriers prior to recombination inside the absorber layer [93]. Free electron and hole pairs are generated inside the perovskite absorber layer in response to light striking a perovskite solar cell. These pairs have a high probability of recombination after traveling a certain distance. Longer carrier lifetimes are associated with longer diffusion lengths, which in turn reduce recombination losses and increase open circuit voltage and short circuit current density, respectively, making perovskite solar cells more efficient.

The carrier lifetime (τ) and saturation current density (J_0) are correlated as [94,95]:

$$J_0 = \frac{qn_i}{2} \sqrt{\frac{D}{\tau}} \quad (5)$$

As we already know from Figure 8, the saturation current density is a function of Br concentration (x) for $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$. Therefore, the carrier lifetime is also a function of Br concentration (x) for $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$, which is calculated from the above Equation (5), and the output response is present in Figure 9 at various trap densities.

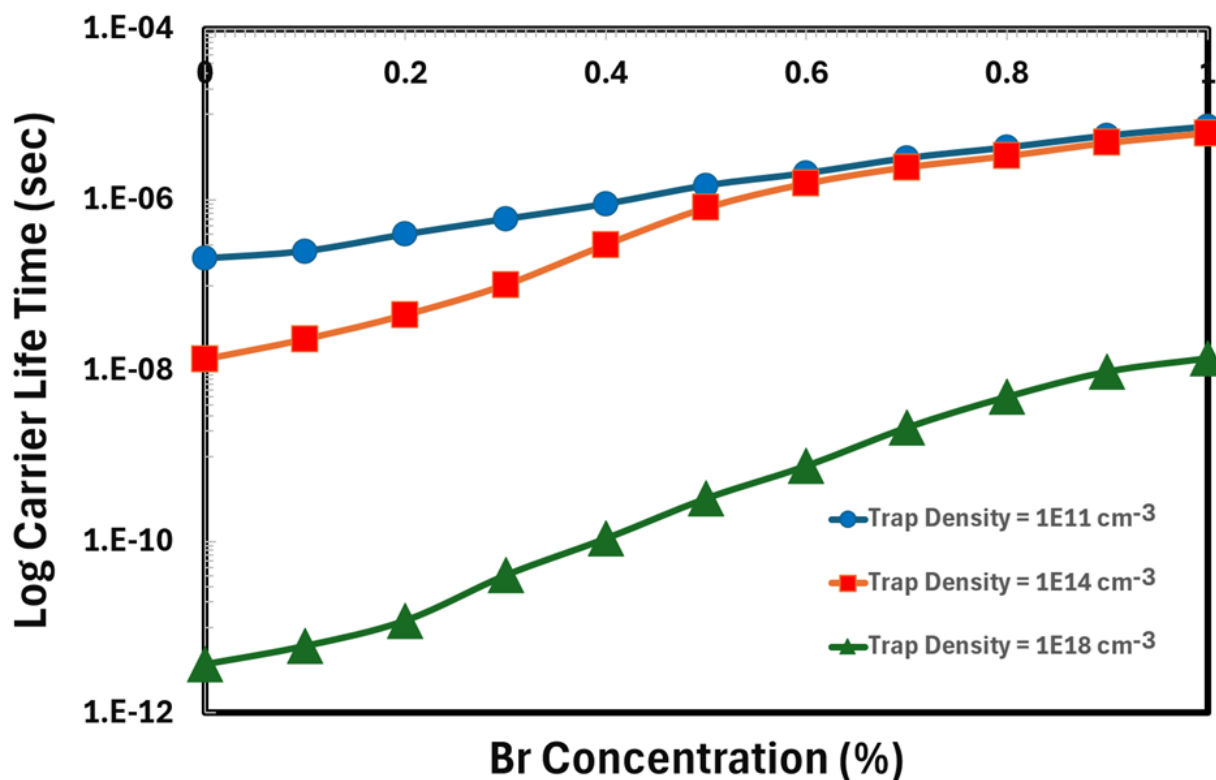


Figure 9. Carrier lifetime (τ) of $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ -based perovskite photovoltaic devices at trap densities of 10^{11} , 10^{12} , and 10^{18} cm^{-3} (as a function of trap density).

The figure shows that the lifetime of carriers is related to how much bromide is in the absorber layer and the number of defects present. Throughout the whole range of Br concentrations, the carrier lifetime for devices with a relatively lower trap density of 10^{11} cm^{-3} is continuously high, on the order of $\sim 10^{-7} \text{ s}$ at $x = 0$ (MAPbI₃), and more or less linearly increases up to $\sim 10^{-6} \text{ s}$ for $x = 1$ (MAPbBr₃). Even at a trap density of 10^{14} cm^{-3} , the carrier lifetime is approximately 10^{-8} s at $x = 0$ (MAPbI₃) and increases quasi-linearly to about 10^{-6} s at $x = 1$ (MAPbBr₃). Both trends are very close after a Br concentration of 0.5, which shows that the recombination dynamics in high-quality films are mostly determined by the intrinsic material properties, rather than the Br concentration in the absorber layer MAPb(Br_xI_{1-x})₃. With an increase in trap density to 10^{14} cm^{-3} inside the absorber layer, there is a slight decrease in carrier lifetime for certain compositions, suggesting that defect-assisted Shockley–Read–Hall recombination starts to be more important. At the maximum defect density of 10^{18} cm^{-3} , the carrier lifetime declines to 10^{-12} to 10^{-9} s , showing the essential dominance of defect-assisted Shockley–Read–Hall recombination. The results suggest that the energy spectrum of the defects may be affected by bromide inclusion, but the existence of a dense and deep level of traps seems to completely nullify its mitigating impact [94–96].

3.7. Effects of Br Concentration on Carrier Diffusion Length (L) and Diffusion Coefficient (D)

The diffusion coefficient (D) is another important parameter used to measure the ease with which free charge carriers can move through a layer with a concentration gradient. Similarly, the carrier diffusion length (L) is the average distance a free carrier travels before the recombination process. The carrier lifetime (τ) is the fundamental link between these two parameters [38]:

$$L = \sqrt{D\tau} \quad (6)$$

where D is calculated through Einstein's relation from Equation (S7).

Figure 10 shows that both carrier diffusion length and diffusion coefficient have very similar trends, monotonically decreasing with increasing bromide concentration. At a Br concentration of $x = 0$ (MAPbI₃), the diffusion length is approximately $0.26 \mu\text{m}$ with a corresponding diffusion coefficient of $0.57 \text{ cm}^2/\text{s}$; however, as the Br fraction increases, both parameters steadily decline, reaching a diffusion length of ~ 0.02 and a diffusion coefficient of $0.26 \text{ cm}^2/\text{s}$ at Br concentration $x = 1$ (MAPbBr₃). The trends might be explained by the fact that the inclusion of bromide causes more free carrier scattering and structural disorder, which in turn increases carrier trapping and decreases mobility. The above relation (Equation (6)) suggests that the degradation in carrier diffusion length is driven mainly by a reduction in diffusion coefficient, rather than a relatively minor change in lifetime. The lowest value of both diffusion coefficient and carrier diffusion length at higher Br concentrations ($x = 1$) indicates that the transport properties are compromised. This may be due to phase segregation or the formation of deep trap states in the presence of a higher concentration of Br in the absorber layer [97].

The aim of including halide in perovskite solar cells is usually to widen the bandgap, and we looked at how this affects open circuit voltage and short circuit current. Through rigorous device simulations, we demonstrate that the synergistic effect of the Br/I ratio on both bandgap and electron affinity may generate non-linear interfacial band offsets, resulting in unforeseen recombination pathways. We observe that interfacial barriers and bulk properties often limit performance when using a full balancing framework. We identify device-specific anomalies, such as unexplained reductions in fill factor that cannot be explained by bandgap scaling, and attribute these to field-dependent charge extraction and trap-assisted recombination at selected interfaces. We distinguish between parameter-driven expectations and actual physical results, thus gaining a better understanding of the

halide-dependent device physics. Our work validates Br/I engineering as a tactical strategy to optimize the overall energy framework, providing design principles for high-efficiency perovskite solar cells.

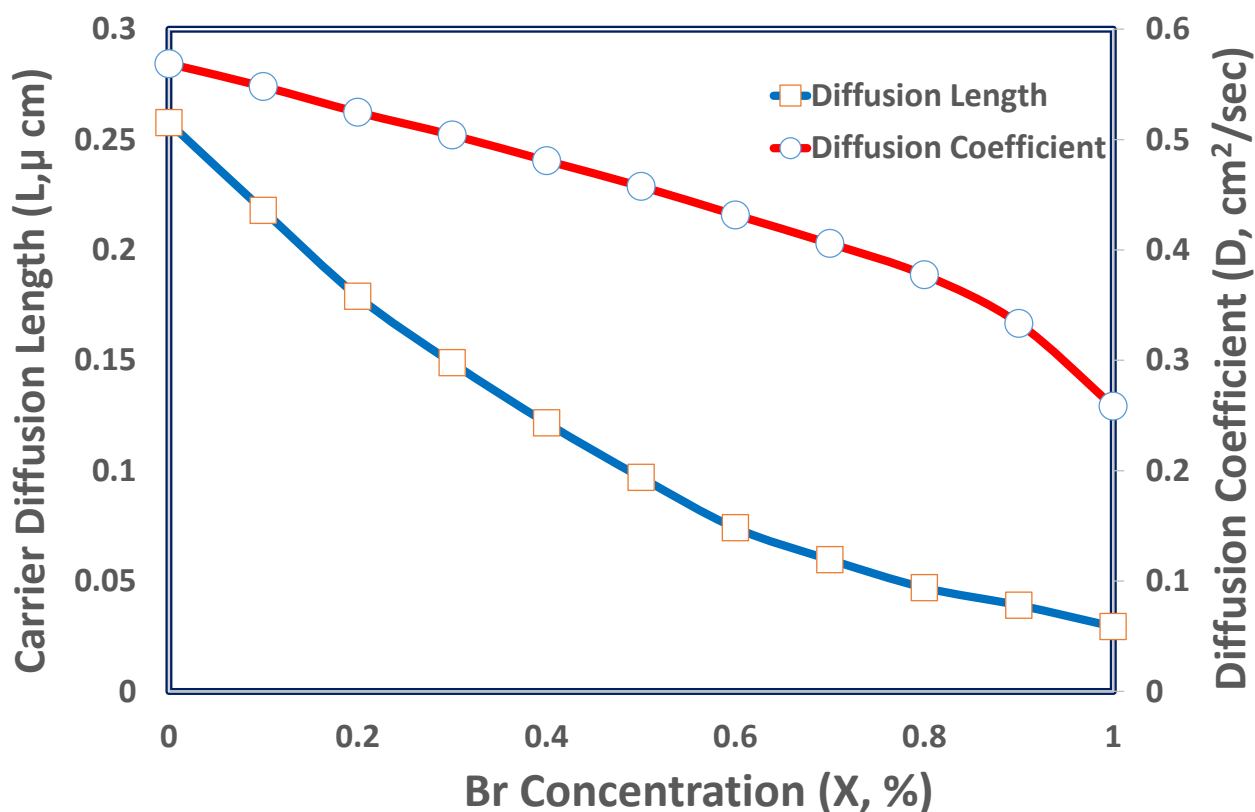


Figure 10. Carrier diffusion length (L) and diffusion coefficient (D) of $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ -based perovskite photovoltaic devices as a function of Br concentration.

3.8. Effects of Temperature on the Photovoltaic Responses of the Devices

The photovoltaic parameter behavior of $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ -based devices as a function of temperature is shown in Figure 11. The figure demonstrates clear temperature-dependent degradation across the measured range of 300 K to 350 K for all devices, especially at lower values of x (Br concentration), with a particular emphasis on the open circuit voltage and fill factor of the devices. As the temperature rises, the open circuit voltage (see Figure 11a) drops gradually in a very similar trend independent of Br concentration (x). This degradation of open circuit voltage with increasing temperature arises from the exponential increase in the reverse saturation current density and causes Shockley–Read–Hall recombination to enhance [98]. In contrast, the short circuit current (see Figure 11b) remains stable throughout the given temperature range (300 to 350 °C) for all concentrations (x) of Br, because at this temperature range the primary factors governing the perovskite solar cells are photocurrent generation, the absorption coefficient, and the energy bandgap. All of these factors exhibit only minor variations (nearly negligible) at this temperature range, suggesting that carrier generation and collection efficiency are largely insensitive to variations within this temperature range. The fill factor shows a slight decline (Figure 11c), while the power conversion efficiency (Figure 11d) decreases correspondingly from 3.1% to 2.5%, reflecting the combined effect of reduced voltage and fill factor at elevated temperatures. These observations may be attributed to enhanced phonon scattering and increased trap-assisted recombination at higher temperatures, which collectively degrade device performance [98–100].

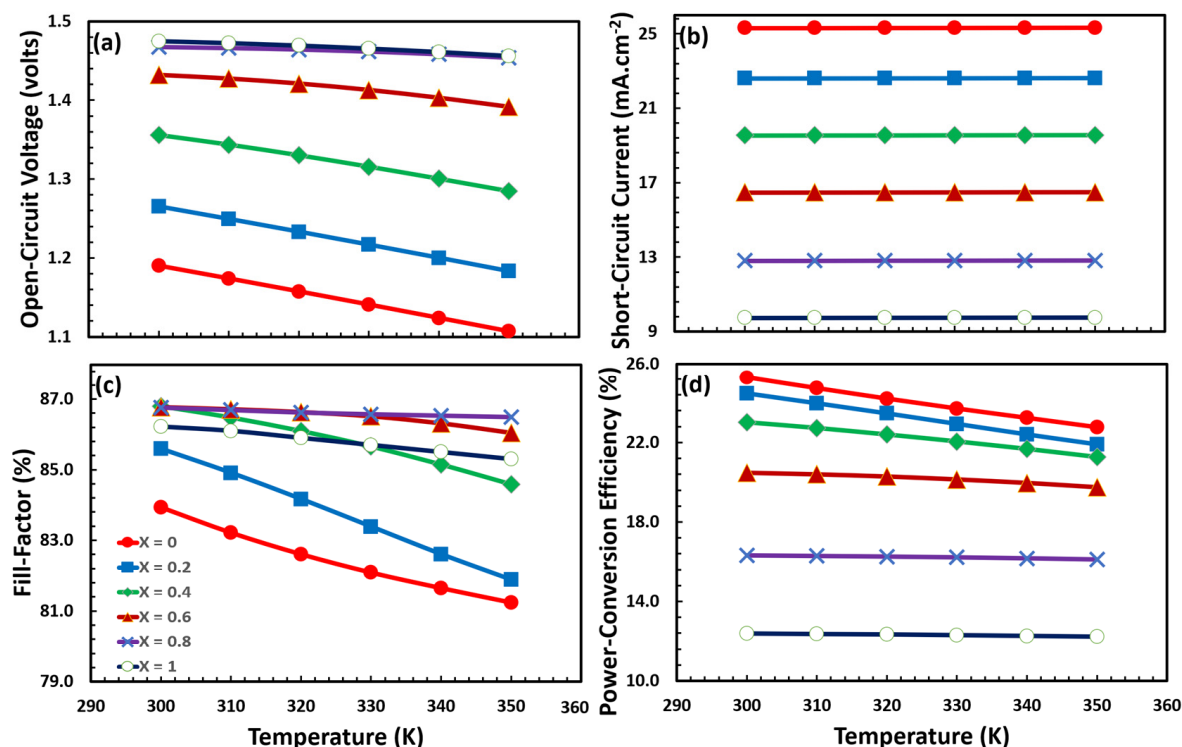


Figure 11. Temperature-dependent photovoltaic performance of MAPb(Br_xI_{1-x})₃-based perovskite solar cells: open circuit voltage (a), short circuit current density (b), fill factor (c), and power conversion efficiency (d) as a function of operating temperature from 300 K to 350 K.

4. Conclusions

While MAPb(Br_xI_{1-x})₃'s compositional flexibility provides a way forward for bandgap engineering, the interplay among halide stoichiometry, thermal stress, carrier dynamics, and defect density is still mostly unknown. By conducting rigorous simulations over the entire Br fraction range, this study systematically maps these interdependencies and uncovers a basic trade-off: as Br enrichment increases, it is important to consider that the bandgap widens. This, in turn, increases open circuit voltage to around 1.5 V while simultaneously decreasing short circuit current from about ~24.5 to about ~9.5 mA·cm⁻² and finally lowering power conversion efficiency from about ~25.5% to about ~12%. Crucially, compositions rich in Br had less temperature-induced degradation of open circuit voltage and fill factor in the 300–350 K range, while absorbers rich in I had stronger photocurrent but greater thermal sensitivity of the fill factor. However, these results are confined to steady-state electrical simulations and do not account for long-term degradation processes, including ion migration, phase segregation, or halide volatilization. As a result, the observed trends should be understood as temperature-dependent performance differences rather than overall thermal stability.

Similarly, carrier transport is decreased in bromide-dominated systems, which is counteracted by an increase in defect tolerance, as seen by the monotonic reduction in extracted carrier lifespan and diffusion length with Br inclusion. Based on these composition-dependent thermal and defect sensitivity asymmetries, we can derive quantitative design principles for customizing mixed halide perovskites, with the possibility that intermediate Br proportions provide the best efficiency/stability compromise. In a broader sense, this model lays the groundwork for understanding temperature-dependent performance trends in mixed halide perovskite photovoltaics, and it directs future experiments toward optimal device designs based on composition.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/nano16150965/s1>. Table S1. List of all investigated devices with varying Br fraction (x) in the perovskite absorber layer, alongside TiO₂ and PEDOT:PSS as ETL (electron-transport layer) and HTL (hole-transport layer). The complete mathematical formulations of the semiconductor transport and recombination models employed in this study, along with the full list of investigated device compositions, are provided in the Supplementary Materials (Equations (S1)–(S15) and Table S1). References [36–48,55,56,94,95] are cited in the Supplementary Materials.

Author Contributions: All coauthors share the same responsibility for conceptualization, methodology, software, validation, formal analysis, investigation, resources, data curation, writing—original draft preparation, writing—review and editing, visualization, supervision, and project administration. All authors have read and agreed to the published version of the manuscript.

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