

Numerical Study of Formamidinium Lead Iodide Perovskite Solar Cells using Solar Cell Capacitance Simulator (SCAPS-1D) Software

Abubakar Sadiq Yusuf

sadiq.yusuf@vuw.ac.nz

Auckland University of Technology

Ramalan Abubakar Muhammad

University of Abuja

Ahmad Alhaji Abubakar

Federal University of Technology

Isah Kimpa Mohammed

Federal University of Technology

Umaru Ahmadu

Federal University of Technology

Kasim Uthman Isah

Federal University of Technology

Zhan Chen

Auckland University of Technology

Maziar Ramezani

Flinders University

Research Article

Keywords: Defect density, Numerical modelling, Optimisation, Perovskite solar cells, Photovoltaic performance, SCAPS-1D

Posted Date: September 22nd, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-10879162/v1>

License: © ⓘ This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

Additional Declarations: No competing interests reported.

Numerical Study of Formamidinium Lead Iodide Perovskite Solar Cells using Solar Cell Capacitance Simulator (SCAPS-1D) Software

Abubakar Sadiq Yusuf^{1,2,4}, Ramalan Abubakar Muhammad³, Ahmad Alhaji Abubakar⁴, Isah Kimpa Mohammed⁴, Umaru Ahmadu⁴, Kasim Uthman Isah⁴, Zhan Chen¹, Maziar Ramezani⁵

¹*School of Engineering, Computer and Mathematical Sciences, Auckland University of Technology, PO Box 92006, Auckland 1142, New Zealand*

²*Robinson Research Institute, Victoria University of Wellington, PO Box 33436, Petone 5046, New Zealand*

³*School of Physical Sciences, Department of Physics, University of Abuja, P.M.B. 117, FCT Abuja, Nigeria*

⁴*School of Physical Sciences, Department of Physics, Federal University of Technology, PMB 65, Minna, Niger State, Nigeria*

⁵*College of Science and Engineering, Flinders University, Sturt Rd., Bedford Park, SA, Australia*

*Corresponding author: sadiq.yusuf@vuw.ac.nz

Abstract:

Perovskite-based solar cells (PSCs) have significantly influenced the photovoltaic industry by outperforming several established solar cell technologies, with power conversion efficiencies (PCEs) already exceeding 23%. Owing to the high costs associated with the experimental development and fabrication of solar cells, researchers have increasingly adopted numerical simulation approaches. Simulation-based optimization offers several advantages, as it is straightforward and cost-effective and enables the prediction of optimal parameters that contribute to the fabrication of solar cells with improved performance. Although PSCs continue to demonstrate promising potential as a viable solar technology, replacing conventional charge transporting layers (CTLs) with inorganic alternatives can enhance long-term device stability and cost-effectiveness. We propose a theoretical study aimed at analysing the performance of Formamidinium Lead Iodide (FAPbI₃)-based PSCs using the SCAPS-1D simulation program. The solar cell is built with a novel and cost-effective planar n-i-p architecture that includes inorganic transport layers. The addition of a thin interface defect layer between the electron transport layer (ETL) and absorber layer significantly improved device performance. Furthermore, a systematic analysis of device parameters was performed, considering critical elements such as working temperature, ETL and absorber thickness, absorber defect density and interface defect layer ($IL_{ETL/At}$). Our optimal device configuration of FTO/SnO₂/IL_{ETL/At}/FAPbI₃/CuI/Ag resulted in an ideal device efficiency of around 25.81%. This research examines a cost-effective architectural design method that prioritizes device efficiency and sustainability.

Keywords: Defect density; Numerical modelling; Optimisation; Perovskite solar cells; Photovoltaic performance; SCAPS-1D.

1. Introduction

Advanced thin-film Perovskite Solar Cell (PSC) technology has achieved a record power conversion efficiency of 25.6% [1], up from its initial value of 3.8% [2]. PSCs are anticipated to rival traditional silicon solar technology in the near future because of their advantageous photovoltaic characteristics [3]. These include efficient absorption of light in the visible spectrum, long distances over which charge carriers can move, a band gap that can be adjusted, the ability to be processed at low temperatures, and ease of manufacturing due to their high tolerance for defects [4-6]. Perovskites possess a distinctive ABX_3 crystal structure, in which A, B, and X represent the monovalent organic cation, bivalent/trivalent metal cation, and anion, respectively. Among the numerous possible ABX_3 combinations, the structural stability and formation of the perovskite phase can be predicted using the Goldschmidt tolerance factor. One of the most promising photovoltaic absorbers is Formamidinium lead iodide (FAPbI₃) perovskite ($A = FA^+$, $B = Pb^{2+}$, $X = I^-$), which has an octahedral factor and is a measure used to determine the coordination number of a metal cation and the halogen anion in a compound [7]. FAPbI₃ has a lower band gap (~ 1.5 eV) and higher thermal stability compared to methylammonium lead iodide (MAPbI₃) [4, 8]. Despite their potential to replace conventional silicon-based solar cell technology, PSCs face long-term stability challenges that hinder their large-scale commercialization [9, 10].

In addition to having an optimized, stable, and low-defect perovskite absorber layer, which is essential for achieving high-efficiency PSCs, CTLs play a crucial role in determining device performance and enhancing long-term stability. The selection of appropriate CTLs requires suitable alignment of the conduction band minimum (CBM) and valence band maximum (VBM) with the energy band structure of the perovskite absorber, thereby facilitating the efficient extraction and collection of photogenerated electrons and holes at their respective electrodes. Furthermore, high electron or hole mobility is an important requirement for CTLs to ensure efficient charge transport within the device. CTLs commonly used in high-performing PSCs are organic Fullerene-based organic ETL, which also degrade under illumination [11]. These considerations, together with existing constraints such as interfacial interactions between working layers, a lack of appropriate deposition/coating processes for large-area devices, expensive deposition tools, and so on, contribute to the lack of PSC deployment on a broad scale. Similarly, (spiro-OMeTAD) or polymeric compounds (PTAA, PCBM, PEDOT: PSS, P3HT) [12-15]. These substances degrade the device's performance over time through a variety of mechanisms. Doped Spiro-OMeTAD, which is widely employed as a hole transporting layer (HTL) in n-i-p solar cells, exhibits thermal degradation at temperatures below 85 °C [16]. Another commonly used HTL in p-i-n structured PSCs is PEDOT:PSS, whose hygroscopic and acidic nature can adversely affect the long-term stability of the device [17]. In this context, substituting widely used organic or polymeric CTLs for PSCs with inorganic alternatives is a viable strategy to extend device lifetimes [18].

N-type semi-conducting oxides such as SnO₂, ZnO and TiO₂ are extensively utilized inorganic ETLs for PSCs [19-21] etc whereas Copper-based semiconductors such as CuI, Cu₂O, CuO, or oxides such as NiO, and others are common alternatives for inorganic HTLs [18]. These inorganic alternatives, in addition to being cost effective, are frequently compatible with a variety of synthesis or film deposition processes [18, 19]. Furthermore, transitioning from chemical or solution processes such as spin coating to physical deposition can reduce the possibility of chemical interaction with the immediate perovskite layer [22].

In recent times, various theoretical simulation software, including Density Functional Theory (DFT), SCAPS, and COMSOL, have been utilized to systematically comprehend the device mechanism of PSCs. This methodical approach can be advantageous in enhancing the practical efficiency of PSCs [23, 24]. The SCAPS-1D software is widely utilized to gain a more comprehensive theoretical understanding of the fundamental mechanisms of solar cells. It also provides a platform for evaluating the potential of various absorber materials, charge transporting layers, and device architectures that can be practically implemented to improve the efficiency and overall performance of photovoltaic devices [25, 26]. SCAPS can be used to analyse various factors that affect cell performance and device stability. These factors include the thickness of different layers (such as ETL, absorber and defect layer), band alignment, the materials used for ETL and HTL, the total defect density of different layers, temperature, doping concentration, and interfacial defect layer.

This article presents an analysis of a novel type of photovoltaic device called an inorganic charge transport layer FAPbI₃-based PSC. The device is developed in a planar (n-i-p) structure and its performance is evaluated using SCAPS-1D simulation software. To investigate, high-performance devices with sustainable stability, we selected inorganic CTLs (SnO₂, CuI) to construct the device. Moreover, the implementation of an interface defect

layer between the ETL/absorber layer resulted in an enhanced operational efficiency of the PSC at lower defects and vis versa. The experimental feasibility of our architectural design is confirmed by the compatibility of all the layers with the perovskite layer [27]. This compatibility has been reported in previous studies on the utilization of these layers in planar structure PSC architecture [27-29]. The device performance was evaluated under various conditions, including temperature variation, thickness of the absorber layer and ETL, absorber defect density and interface defect layer.

By optimizing operating temperature (T-310 K), ETL/absorber layer thicknesses, and considering realistic values for absorber defect density (N_t - $3.162 \times 10^{13} \text{ cm}^{-3}$) and interface defect density layer ($IL_{\text{ETL/AT}}$ - $1 \times 10^{15} \text{ cm}^{-3}$) our inorganic transporting layer PSC achieved a low efficiency of 12.99%. This was accompanied by J_{SC} (12.19 mA/cm^2), V_{OC} (1.259 V), and FF (84.27%). Under nearly perfect conditions, with absorber defect density and interface defect layer of N_t - $1 \times 10^{12} \text{ cm}^{-3}$ and $IL_{\text{ETL/AT}}$ - $1 \times 10^8 \text{ cm}^{-3}$, optimum thicknesses 300 and 500 nm ETL and absorber respectively and a temperature of 300 K, the n-i-p planar structured PSC achieved an exceptional efficiency of 25.81%. The cell also exhibited a high short-circuit current density (J_{SC}) of 23.87 mA/cm^2 , a high open-circuit voltage (V_{OC}) of 1.28 V, and a high fill factor (FF) of 84.20%.

2. Simulation Methodology

The SCAPS-1D is a powerful one-dimensional simulation software developed by the Department of Electronics and Information Systems at the University of Gent in Belgium. This software facilitates the design of various cell structures, allowing users to model up to seven different layers. Figures 1 illustrate the layer architecture and definition panel of Perovskite solar cells using SCAPS-1D, respectively.

2.1 Simulation Tool-SCAPS-1D

SCAPS-1D calculates essential performance parameters such as I - V characteristics, carrier density, band diagram, current density, quantum efficiency, and more. The simulation involves solving differential equations, including Poisson's equation representing electrostatic potential, electron and hole continuity equations, transport equations, and diffusion lengths.

- **Poisson's equation**

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{\partial E}{\partial x} = -\frac{\rho}{\epsilon_s} = -\frac{q}{\epsilon_s} [p - n + N_D^+(x) - N_A^-(x) \pm N_t(x)] \quad (1)$$

where N^+ , N^- , and N_t represent the densities of ionized donors, ionized acceptors, and trap states, respectively; ψ denotes the electrostatic potential, q is the elementary charge, and ϵ_s represents the static relative permittivity of the medium [30]. The steady-state electron and hole continuity equations are expressed as follows:

- **Continuity Equations for electron and hole**

$$\frac{\partial j_n}{\partial x} + G - R_n(n, p) = 0 \quad (2)$$

$$-\frac{\partial j_p}{\partial x} + G - R_p(n, p) = 0 \quad (3)$$

where R_n and R_p denote the net recombination rates of electrons and holes, respectively, G represents the electron-hole pair generation rate, and j_n and j_p correspond to the electron and hole current densities, respectively. The electron and hole current densities are described by the following equations:

- **Transport Equations**

$$j_n = q\mu_n E + qD_n \frac{\partial n}{\partial x} \quad (4)$$

$$jp = qp\mu_n E + qD_p \frac{\partial p}{\partial x} \quad (5)$$

where q denotes the elementary charge, μ_n and μ_p represent the electron and hole mobilities, respectively, while D_n and D_p correspond to the electron and hole diffusion coefficients, respectively.

- **Diffusion Length**

$$L_n = \sqrt{D_n \tau_n} \quad (6)$$

$$L_p = \sqrt{D_p \tau_p} \quad (7)$$

The program can simulate solar cells under different conditions, providing comprehensive insights into their fundamental properties, including the simulations provide information on the energy band diagram, charge-carrier generation and recombination rates, external quantum efficiency, current density, and J - V characteristics, including the short-circuit current density, open-circuit voltage, fill factor, and power conversion efficiency. In this study, the simulations were performed under Standard Test Conditions (STC), using an Air Mass (AM) 1.5G solar spectrum, an irradiance of 1000 W/m², and a temperature of 300 K.

2.2 Device modelling

The Solar Cell Capacitance Simulator, also known as SCAPS-1D, is a theoretical simulation tool that was first created by a team of researchers from the department of Electronics and Information Systems (ELIS) at the University of Gent in Belgium. While initially designed for CdTe and CIGS based solar families [31], SCAPS has become a widely adopted simulation platform for modelling various photovoltaic device architectures, including PSCs, dye-sensitized solar cells (DSSCs), silicon-based solar cells, and tandem solar cells [32-34]. The user can analyse the performance of a solar cell by considering various parameters such as Key parameters include the bandgap, electron affinity, donor and acceptor densities, defect density and energy levels, recombination mechanisms such as direct band-to-band, Auger, and Shockley-Read-Hall (SRH) recombination, operating temperature, tunnelling mechanisms, metal work function, and flat-band conditions. These parameters play a critical role in determining the proper operation and overall performance of the solar cell. Furthermore, it functions as a platform for investigating new device configurations or semiconducting materials that may be used as CTLs/absorber layers. It also allows for the identification of any underlying device mechanisms that can be experimentally applied to enhance the performance of solar cells.

This work used a planar structure n-i-p device configuration to replicate the performance of a PSC. The device consisted of FAPbI₃ as the light absorber layer, SnO₂ as the electron transporting layer, CuI as the hole transporting layer and Silver (Ag) electrode. FTO functioned as the upper electrode, serving as a transparent window for light to penetrate. The simulated solar cell consists of a device configuration with the layers FTO/SnO₂/IL_{ETL/At}/FAPbI₃/CuI/Ag. This structure is shown in Fig. 1. The present study utilizes widely available starting materials, namely SnO₂ and CuI for the CTLs, and IL_{ETL/At} for the interface defect layer. These materials may be readily synthesized in the laboratory using solution-based techniques as described in previous publications [35-38]. To provide a more accurate comparison, let's use the example of high purity PCBM, which is often employed as an electron transport layer in planar structure perovskite solar cell configurations. Surprisingly, the cost of this material is even higher than that of an equivalent amount of gold! Nevertheless, our suggested design of inorganic CTLs while maintaining device performance. Utilizing inorganic layers that possess chemically inert qualities may effectively prevent deterioration over long periods of time, hence increasing the lifespan of PSCs. Hence, we underline that our suggested approach meets the two requirements of being cost-effective and reliable at the same time. The parameters for each layer have been summed up in Table 1 and 2. The device's performance was enhanced by adjusting several parameters, including the thickness of the accompanying layers, the defect density of the absorber layer (Nt) and the interface defect layer and the operating temperatures (T). These parameters were crucial in determining the maximum achievable efficiency and overall performance of the device.

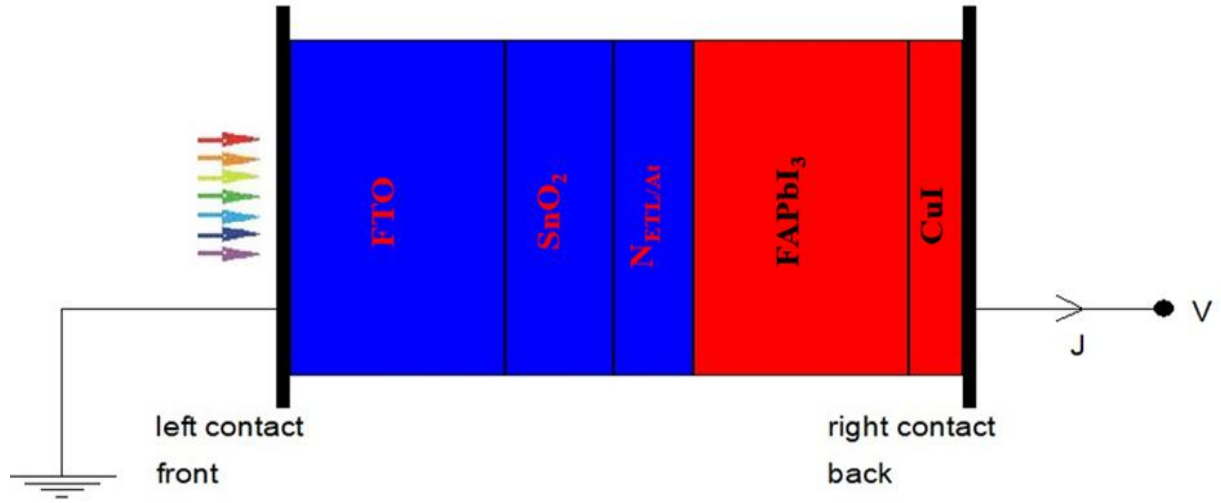


Figure 1. Perovskite solar cells layer architecture with SCAPS-1D.

Table 1

List of simulation parameters for PSC.

Parameters	FTO [39, 40]	SnO ₂ [41, 42]	Interface defect layer (IL _{ETL/AI}) [43]	FAPbI ₃ [44]	CuI [42]
Thickness (nm)	400	100	10	100	100
Band gap (eV)	3.6	3.5	1.5	1.51	2.98
Electron affinity (eV)	4.2	4.2	3.9	4.0	2.1
Dielectric permittivity	10	10	6.5	6.6	6.5
CB effective density of states (cm ⁻³)	2.10 ¹⁸	2.2×10 ¹⁸	2	1.2×10 ¹⁹	2.8×10 ¹⁹
VB effective density of states (cm ⁻³)	1.8×10 ¹⁹	1.9×10 ¹⁹	2	2.9×10 ¹⁸	2.0×10 ¹⁹
Thermal velocity of electrons (cm/s)	10 ⁷	10 ⁷	10 ⁷	10 ⁷	10 ⁷
Thermal velocity of holes (cm/s)	10 ⁷	10 ⁷	10 ⁷	10 ⁷	10 ⁷
Electron mobility (cm ² /Vs)	50	40	2	2.7	10 ⁻⁴
Hole mobility (cm ² /Vs)	75	25	2	1.8	40
Shallow donor density N_D (cm ⁻³)	10 ¹⁹	10 ¹⁸	10 ¹⁷	0	0
Shallow acceptor density N_A (cm ⁻³)	0	0	0	1.3×10 ¹⁶	10 ¹⁸
Defect density N_t (cm ⁻³)	10 ¹⁵	10 ¹⁵	5×10 ¹¹	3.162×10 ¹⁵	10 ¹⁵

Table 2

List of parameter values of the device interface

Parameters	FAPbI ₃ defect [45, 46]	Defect layer [45, 46]
Defect type	Neutral	Neutral
Capture cross section for electrons (cm ²)	1.2×10^{-13}	1×10^{-19}
Capture cross section for holes (cm ²)	1.2×10^{-13}	1×10^{-19}
Energetic distribution	Single	Single
Energy level with respect to E_v (eV)	0.600	0.600
Characteristic energy eV)	0.1	0.1
Total density (cm ⁻³)	1×10^{12}	1×10^{12}

3. Results and Discussion

3.1 Influence of Working Temperature

The operational temperature is a critical external variable that significantly impacts the efficiency of PSCs. Halide perovskites are often associated with stability problems, with temperature being one of the factors that contribute to the deterioration of the perovskite absorber, resulting in reduced device performance. While SCAPS cannot directly measure the degradation dynamics of the PSC at various operational temperatures, it may provide insight into how device characteristics vary when exposed to varied operating temperatures. We therefore simulated the device (ETL- 100 nm, absorber - 100 nm, HTL- 100 nm, absorber N_t - $3.162 \times 10^{16} \text{ cm}^{-3}$) investigate the effect of temperature on the solar cell devices at various temperatures ranging from 300 K to 350 K in increments of 10 K, while subjecting it to AM 1.5 sun radiation conditions. Based on the information provided in Figure 2 (a-d), it is evident that, with the increase in operating temperature, all device metrics exhibit a consistent reduction. This includes parameters such as V_{OC} , J_{SC} and FF. In general, the PSC saw a decrease in efficiency as the temperature rose, perhaps because to the occurrence of more recombination events caused by higher thermal vibrations. The device achieved a relatively low PCE of 12.94%, with a J_{SC} of 12.192 mA/cm², an V_{OC} of 1.259 V, and a FF of 84.27%.

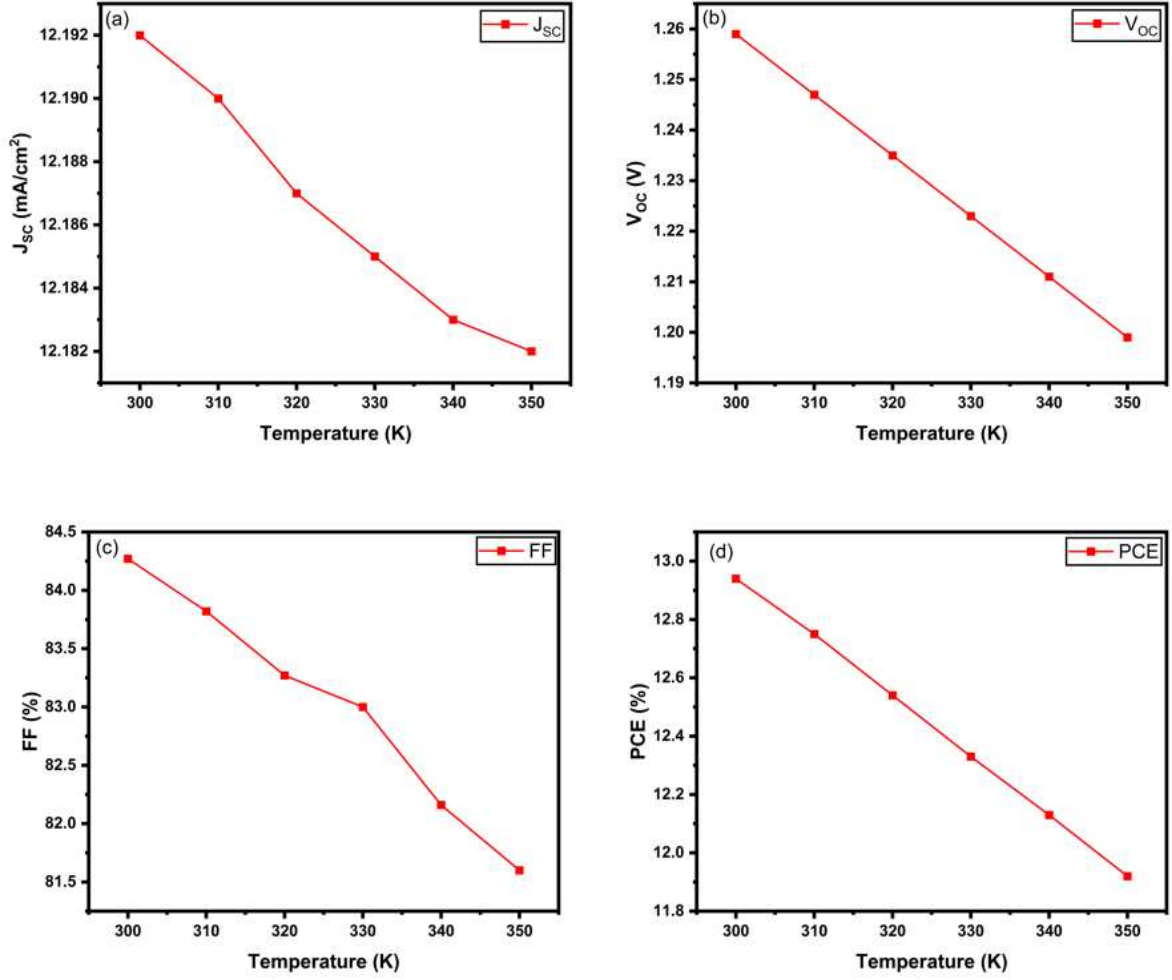


Figure 2. Parameter varied for temperature (a) J_{sc} (b) V_{oc} (c) FF and (d) PCE.

3.2 Influence of ETL Thickness Variation

SnO_2 is often used as an n-type semiconductor in a certain sort of solar cell configuration called n-i-p PSC. It is typically used as an ETL. This information is supported by the studies conducted by [37, 47]. Nevertheless, there are experimental studies documenting the application of SnO_2 to a planar p-i-n structure as well [38, 48]. This allows for the cost-effective production of PSC devices, replacing the need for expensive polymeric compounds such as PCBM. In our device simulation, we have used SnO_2 as the ETL. Using a properly aligned SnO_2 with the absorber ensures that there is little recombination at the interface between the absorber and the ETL, which in turn improves the performance of the device.

To examine how changes in the thickness of the ETL impact the performance of the device, we conducted simulations on a PSC. The simulations were carried out at an optimized temperature of 300 K, absorber thickness of 500 nm over a range of thickness varying from 100 - 1000 nm in an increment of 100 nm under AM 1.5 solar radiation conditions. The optimal thickness of the ETL layer was set at 300 nm. Based on the observations made in Figure 3(a-d), all the parameters (J_{sc} , V_{oc} , FF and PCE) follow a similar pattern. The variation in ETL thickness shows an almost negligible reduction in all device performance parameters, with changes occurring only in the third or fourth decimal place when the ETL thickness reaches 300 nm. Therefore, a very thin ETL may not provide an effective barrier against minority charge carriers at the perovskite/ETL interface, leading to increased charge-carrier recombination. Such recombination can reduce the J_{sc} and, consequently, the overall power conversion efficiency of the device. Therefore, we have selected a thickness of 300 nm as the optimal ETL for further simulations.

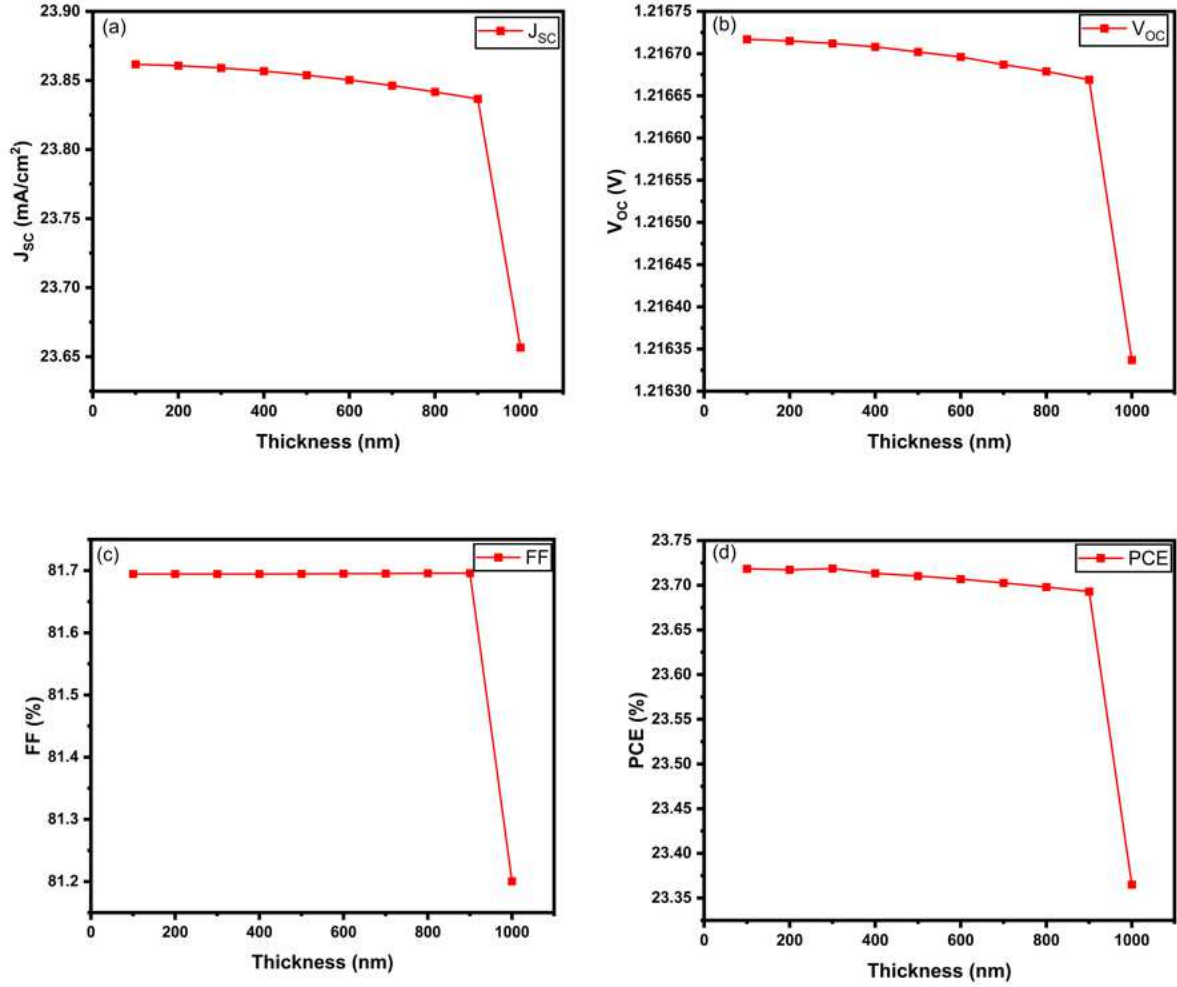


Figure 3. Parameters of SnO₂ ETL thickness variation on the photovoltaic: (a) J_{sc} , (b) V_{oc} , (c) FF, and (d) PCE

3.3 Influence of Perovskite Defect Density (N_t)

Polycrystalline perovskite films are susceptible to several inherent and external flaws that often diminish their efficiency as solar cells. Although perovskites are naturally recognized for their ability to tolerate defects because of their distinctive electrical structure, the methods often used for producing perovskite thin films via solution processing inadvertently result in the introduction of defects. The shallow-defect states, which are positioned around the borders of the valence band or conduction band, are regarded relatively benign for the PSCs [49]. These states include the capture and release of charge carriers, but they do not impact the overall carrier concentration. Conversely, defects positioned near the center of the energy bandgap in perovskites are referred to as deep-level traps. These traps can collect both types of charge carriers, namely electrons and holes. Carriers that are stuck at these locations with significant defects are finally eliminated by a process called non-radiative recombination. This mechanism is responsible for the depletion of photogenerated carriers in PSCs [49]. The trap-assisted non-radiative recombination routes in metal halide perovskites may be categorized as Shockley-Read-Hall (SRH) recombination and Auger recombination. However, it has been shown that SRH recombination is the primary mechanism in perovskites with defect concentrations below 10^{17} cm^{-3} [50].

This defects in the active layer stands out as a crucial parameter significantly impacting device performance. Elevated defect concentrations in the absorber layer led to increased recombination, attributed to the formation of pinholes, accelerated film degradation, reduced stability, and an overall decline in device performance [51]. The defect density (N_t) plays a pivotal role in the efficiency of the PSC (Al-Asbahi et al., 2020). A higher N_t signifies a greater quantity of trap layers within the perovskite film of the cell [52]. These trap states induce an increase in non-radiative recombination and pose obstacles to the movement of charge particles [53], both contributing to a

reduction in the efficiency of the photovoltaic (PV) cell. The heightened defect density diminishes the carrier lifetime (τ) of the charge carriers, accelerating the recombination rate, subsequently leading to a reduction in absorption length (L) (Equation 3). As N_t increases, the absorption length of the layer decreases [27].

The simulations were carried out at an optimized temperature of 300 K, ETL and absorber thickness of 300 and 500 nm, $IL_{ETL/At}$ 10^7 cm^{-3} and N_t varied from 10^8 to 10^{20} cm^{-3} under AM 1.5 solar radiation conditions. The defect at absorber is assumed neutral, with a single defect energy distribution situated 0.6 eV above EV and an initial N_t of 10^8 cm^{-3} . Figure 4 (a-d) shows how changing the N_t from 10^8 to 10^{20} cm^{-3} affects device characteristics. N_t levels below 10^{11} cm^{-3} did not substantially impact device performance. However, N_t levels over 10^{17} cm^{-3} resulted in a slight decrease in efficiency, the device performance changed from a PCE of 23.71%, a J_{SC} of 23.862 mA/cm^2 , an V_{OC} of 1.216 V, and an FF of 81.6942% to a PCE of 21.49%, a J_{SC} of 23.623 mA/cm^2 , a V_{OC} of 1.238 V, and an FF of 76.75%.

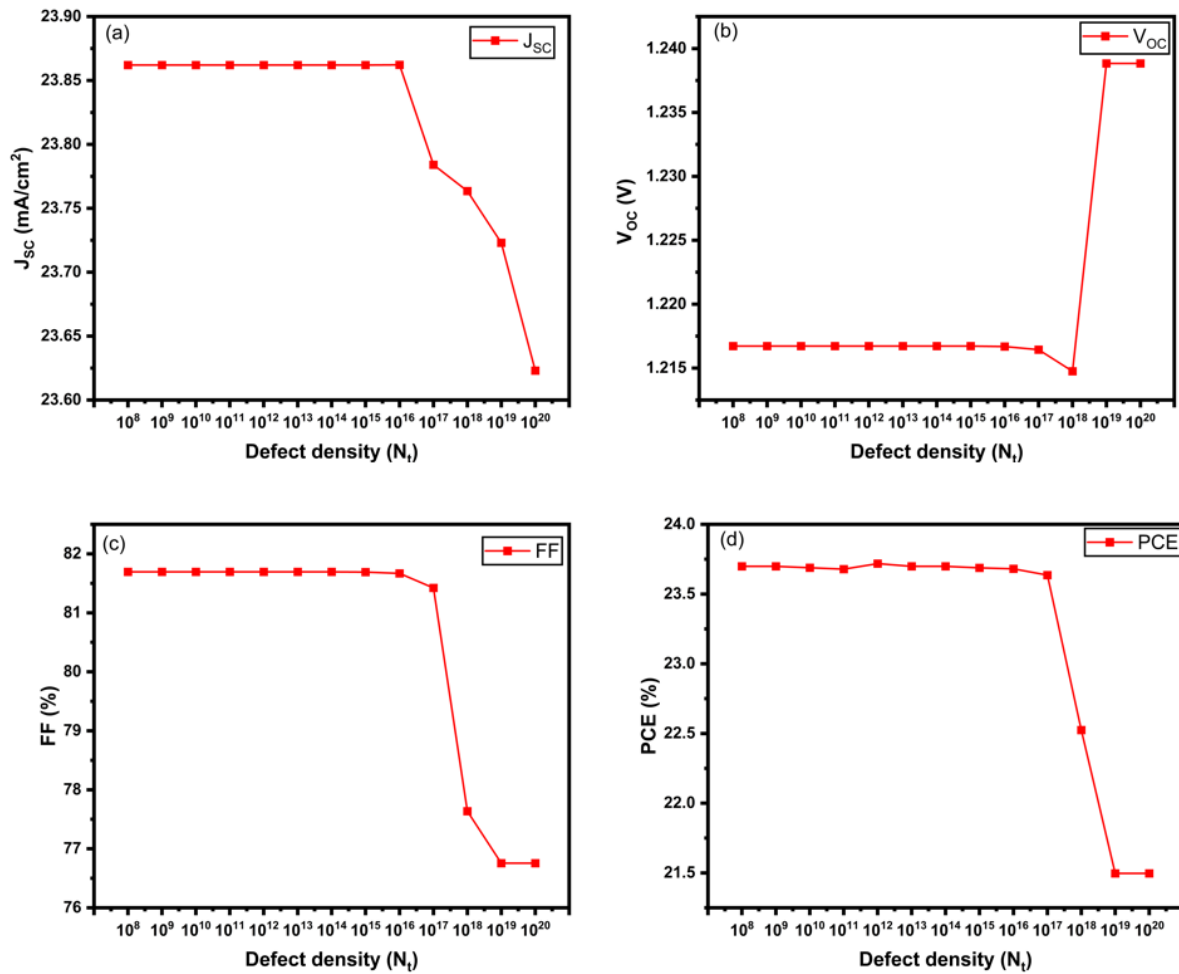


Figure 4. Parameter varied for perovskite defect density (a) J_{SC} (b) V_{OC} (c) FF and (d) PCE.

3.4 Influence of Absorber Thickness Variation

To ensure optimal device performance, it is crucial to choose an absorber with the ideal thickness (500 nm). This absorber should be able to absorb the greatest amount of light energy and produce enough charge carriers, all while avoiding any increase in the device's overall resistance or hindering the separation of carriers. Therefore, the first stage of our simulation involves optimizing the thickness of the absorber layer. Formamidinium lead iodide (FAPbI₃) is used as the photosensitive layer in this case. The band gap of FAPbI₃ is precisely 1.51 eV. The simulation was carried out at an optimized temperature of 300 K, ETL thickness of 300 nm, $IL_{ETL/At}$ 10^7 cm^{-3} , N_t 10^8 cm^{-3} and absorber thickness was varied from 100 – 1000 nm under AM 1.5 solar radiation conditions to

optimize the performance, the absorber layer with a thickness of 500 nm, as shown in Fig. 5(d), exhibited the best device performance. Based on the information provided in Figure 5(a-d) it is evident that the J_{SC} values were originally low for thin absorber layers. This suggests that there was inadequate production of electron-hole pairs inside the layer. The values of J_{SC} and efficiency both improve when the thickness is raised, reaching their greatest values for an absorber thickness of 500 nm. Subsequent increments in the thickness of the layer led to decreased values of J_{SC} , FF, and efficiency, ultimately causing a decline in the performance of the device. The observed trend for absorber layers thicker than 500 nm may be attributed to an elevation in the internal resistance of the absorber [54]. This is caused by the accumulation of photo-generated carriers, which ultimately collide and recombine before being collected by the electrodes. The optimum thickness of 500 nm achieved the PCE of 24.62%, a J_{SC} of 25.104 mA/cm², an V_{OC} of 1.208 V, and a FF of 81.200%

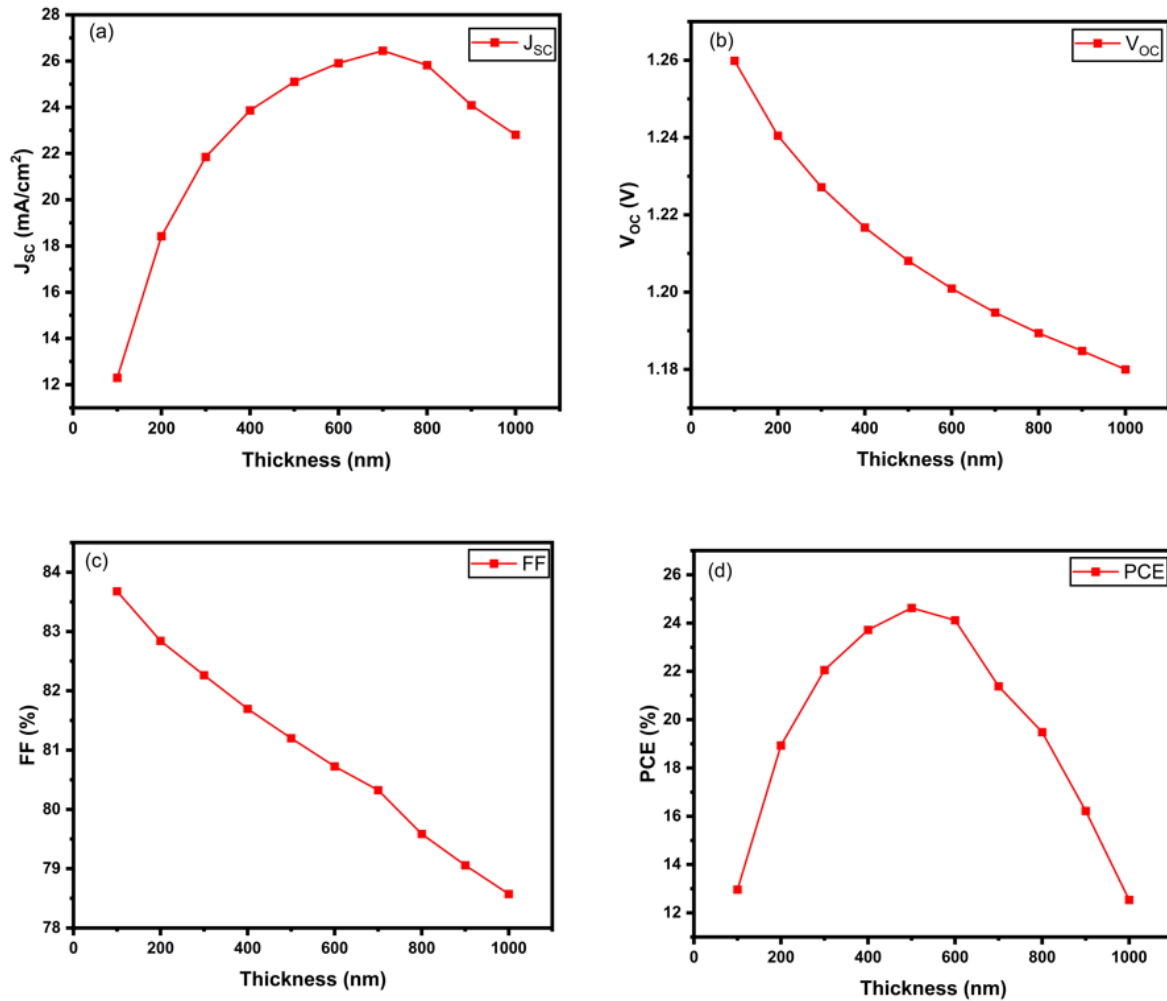


Figure 5. Parameter varied for FAPbI₃ thickness (a) Current density (J_{SC}) (b) Open circuit voltage (V_{OC}) (c) Fill factor (FF) and (d) Power conversion efficiency (PCE).

3.5 Influence of interface defect layer ($IL_{ETL/AI}$)

The Interface defect layer makes direct contact with the ETL and absorber, hence it plays a crucial role in device performance. To achieve crystallinity, the ETL and absorber layer are typically solution treated and then annealed at a certain temperature range. Non-optimal conditions can lead to the formation of defects within the absorber layer and at the absorber/ETL interface, which are nearly unavoidable. The built-in electric field resulting from band alignment at the interface facilitates the selective transport and extraction of charge carriers, particularly electrons at the ETL/absorber interface. However, this process is hindered by high defect density at the ETL/absorber interface. To determine the influence of Interface defect layer on our n-i-p structured device, we investigated the change in device characteristics by increasing ($IL_{ETL/AI}$) from 10^7 to 10^{20} cm⁻³ at the interface

defect layer with optimized temperature of 300 K, ETL/absorber thicknesses of 300 and 500 nm and N_t 10^8 cm^{-3} under AM 1.5 solar radiation conditions to optimize the performance. The defect at $\text{IL}_{\text{ETL}/\text{At}}$ is assumed neutral, with a single defect energy distribution situated 0.6 eV above EV. Figure 6 (a-d) shows how changing the $\text{IL}_{\text{ETL}/\text{At}}$ from 10^7 to 10^{20} cm^{-3} affects device characteristics. $\text{IL}_{\text{ETL}/\text{At}}$ levels below 10^{12} cm^{-3} did not substantially impact device performance. However, $\text{IL}_{\text{ETL}/\text{At}}$ levels over 10^{13} cm^{-3} resulted in a considerable decrease in efficiency, from PCE of 23.717%, a J_{SC} of 23.860 mA/cm^2 , an V_{OC} of 1.216V, and a FF of 81.694% to a PCE of 12.13%, a J_{SC} of 22.790 mA/cm^2 , an V_{OC} of 0.829V, and a FF of 64.190%.

The findings indicates that $\text{IL}_{\text{ETL}/\text{At}}$ is more negatively impacted by defect states compared to absorber defect density N_t . Similar observations were reported by Huang et al. (2016), Lin et al. (2021), and Jannat et al. (2021), demonstrating that the interface located at the front, or illuminated side, of the PSC has a more pronounced influence on overall device performance [55-57]. Since we simulated a planar n-i-p structured PSC with the ($\text{SnO}_2/\text{IL}_{\text{ETL}/\text{At}}/\text{FAPbI}_3$) on the back side, the findings are consistent with earlier publications. As light radiations reach the absorber from the front, they may be absorbed closer to the ETL side (rather than in the center), resulting in more electron pairs closer to the front.

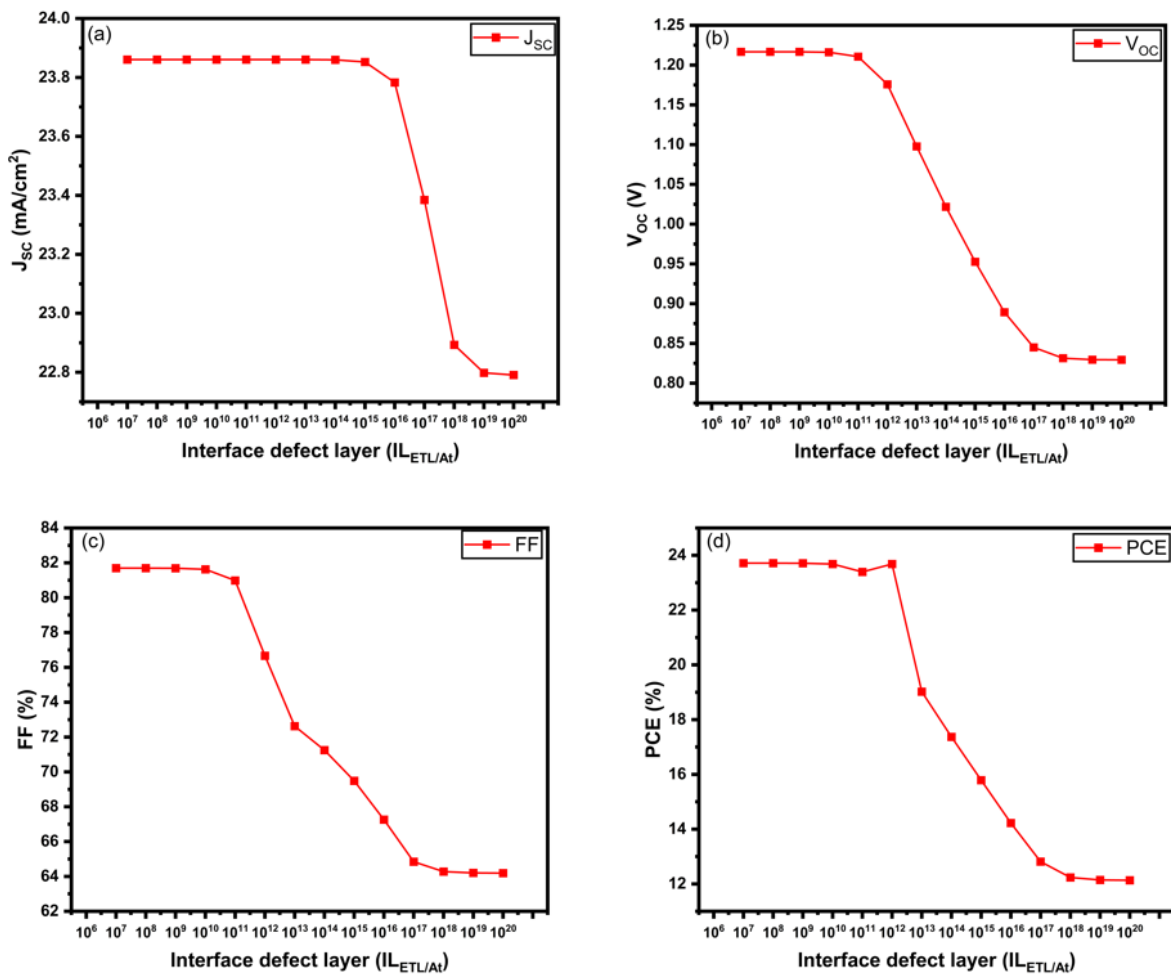


Figure 6. Parameter varied for Interface defect layer ($N_{\text{ETL}/\text{At}}$) (a) J_{SC} (b) V_{OC} , (c) FF and (d) PCE.

3.6 Performance of the Optimised Device

Figure 7 illustrates the characteristic curve of the optimised device. The parameters set for optimisation include a working temperature of 300K, ETL and Perovskite thickness of 300 and 500 nm respectively, a Perovskite defect density of 10^{12} cm^{-3} , and Interface defect layer 10^8 cm^{-3} . The optimised device demonstrated impressive performance metrics, yielding a PCE of 25.81%, a J_{SC} of 23.877 mA/cm^2 , an V_{OC} of 1.283 V, and FF of 84.20%. These results offer valuable insights for researchers engaged in the experimental development of solar cells based

on FAPbI₃ are more stable resulting in high power conversion efficiency, making it a promising material for use in PSCs providing a pathway towards achieving high performance in such devices.

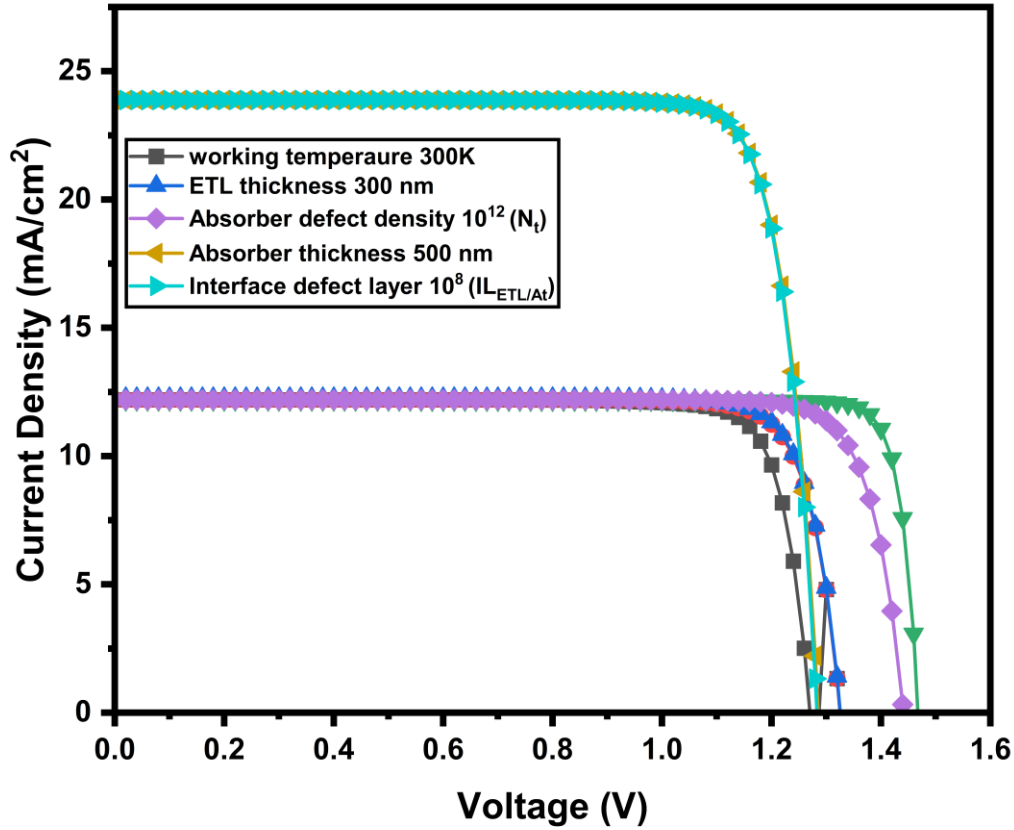


Figure 7. J-V curve of the optimised simulated PSC.

4. Conclusion

In this study, we conducted a theoretical analysis of a novel perovskite solar cell of device architecture (FTO/SnO₂/IL_{ETL/At}/FAPbI₃/CuI/Ag) cost-effective, inorganic charge transporting layer-based FAPbI₃-Perovskite solar cell in a planar configuration. We demonstrate that employing optimum layer thicknesses for the ETL and absorber as well as the addition of an optimized perovskite defect density (N_t) and interface defect layer (IL_{ETL/At}), the PSC efficiency can be increased from 12.19% to over 25.81%. Furthermore, a thorough understanding of the interdependence of absorber thickness and defect density (N_t) on PSC performance reveals that to achieve high efficiencies, perovskite absorber films with a high defect density should be comparatively thinner, whereas absorber layers containing fewer defects can accommodate greater thicknesses to achieve improved device performance. This behaviour can be attributed to the diffusion length of photogenerated charge carriers and the probability of Shockley–Read–Hall (SRH) recombination, both of which are strongly dependent on the absorber defect density (N_t), a key factor governing PSC performance. In addition, the influence of the interfacial defect layer (IL_{ETL/At}) located between the ETL and the absorber layer on the photovoltaic characteristics of the solar cell was investigated. Our FAPbI₃-perovskite solar cell performed well under AM1.5 solar illumination, with PCE of 25.81%, J_{SC} of 23.87 mA/cm², V_{OC} of 1.283 V, and FF of 84.20%. The device had low absorber defect density (1×10^{12} cm⁻³), low interface defect layer (1×10^8 cm⁻³), and 300 K operating temperature. This study demonstrates the ability of an inorganic charge transporting layer FAPbI₃-based PSC to achieve higher efficiencies and stability

while remaining cost-effective by replacing conventionally used expensive CTLs with low-cost inorganic metal oxide layers like SnO₂ and CuI.

Acknowledgements

The first author would like to thank the Tertiary education trust fund (Tetfund) of Nigeria for their financial support.

Credit authorship contribution statement

ASY: Conceptualization, Methodology, Writing - original draft, Writing - review & editing, Resources. **RAM:** Visualization, Writing - review & editing. **AAA:** Visualization, Writing - review & editing **UM:** Visualization, Writing - review & editing. **IMK:** Visualization, Writing - review & editing. **KUI:** Visualization, Writing - review & editing. **ZC:** Supervision, Writing - review & editing. **MR:** Supervision, Writing - review & editing.

Funding

The study was funded by the Tertiary Education Trust Fund (Tetfund) with funding number TETF/ES/UNIV/NIGER STATE/ TSAS/2020

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work presented in this study.

Data Availability

The data supporting the findings of this study will be made available upon reasonable request.

Declarations

Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Competing interests

The authors declare no competing interests

Clinical trial registration

Not applicable. This study does not involve a clinical trial.

References

- [1]. Min, H., et al., *Perovskite solar cells with atomically coherent interlayers on SnO₂ electrodes*. Nature, 2021. **598**(7881): p. 444-450.DOI: <https://doi.org/10.1038/s41586-021-03964-8>.
- [2]. Kojima, A., et al., *Organometal halide perovskites as visible-light sensitizers for photovoltaic cells*. Journal of the american chemical society, 2009. **131**(17): p. 6050-6051.DOI: doi.org/10.1021/ja809598r.
- [3]. Olaleru, S.A., et al., *Perovskite solar cells: The new epoch in photovoltaics*. Solar Energy, 2020. **196**: p. 295-309.DOI: <https://doi.org/10.1016/j.solener.2019.12.025>.
- [4]. Amat, A., et al., *Cation-induced band-gap tuning in organohalide perovskites: interplay of spin-orbit coupling and octahedra tilting*. Nano letters, 2014. **14**(6): p. 3608-3616.DOI: doi.org/10.1021/nl5012992.

- [5]. Gholipour, S. and M. Saliba, *Bandgap tuning and compositional exchange for lead halide perovskite materials*, in *Characterization Techniques for Perovskite Solar Cell Materials*. 2020, Elsevier. p. 1-22.
- [6]. Jang, D.M., et al., *Reversible halide exchange reaction of organometal trihalide perovskite colloidal nanocrystals for full-range band gap tuning*. Nano letters, 2015. **15**(8): p. 5191-5199.DOI: doi.org/10.1021/acs.nanolett.5b01430.
- [7]. Nayak, M., et al., *A roadmap towards stable perovskite solar cells: prospective on substitution of organic (A) & inorganic (B) cations*. Journal of Materials Science: Materials in Electronics, 2021. **32**(14): p. 18466-18511.DOI: https://doi.org/10.1007/s10854-021-06431-2.
- [8]. Zheng, Z., et al., *Development of formamidinium lead iodide-based perovskite solar cells: efficiency and stability*. Chem Sci, 2022. **13**(8): p. 2167-2183.DOI: 10.1039/d1sc04769h.
- [9]. Rong, Y., et al., *Challenges for commercializing perovskite solar cells*. Science, 2018. **361**(6408): p. eaat8235.DOI: 10.1126/science.aat8235.
- [10]. Duan, L. and A. Uddin, *Defects and stability of perovskite solar cells: a critical analysis*. Materials Chemistry Frontiers, 2022. **6**(4): p. 400-417.DOI: https://doi.org/10.1039/D1QM01250A.
- [11]. Akbulatov, A.F., et al., *Effect of Electron-transport material on light-induced degradation of inverted planar junction perovskite solar cells*. Advanced Energy Materials, 2017. **7**(19): p. 1700476.DOI: doi.org/10.1002/aenm.201700476.
- [12]. Li, S., et al., *A brief review of hole transporting materials commonly used in perovskite solar cells*. Rare Metals, 2021. **40**(10): p. 2712-2729.DOI: 10.1007/s12598-020-01691-z.
- [13]. Yang, G., et al., *Recent progress in electron transport layers for efficient perovskite solar cells*. Journal of Materials Chemistry A, 2016. **4**(11): p. 3970-3990.DOI: 10.1039/c5ta09011c.
- [14]. Jiang, Q., X. Zhang, and J. You, *SnO₂: a wonderful electron transport layer for perovskite solar cells*. Small, 2018. **14**(31): p. 1801154.DOI: https://doi.org/10.1002/smll.201801154.
- [15]. Xu, H., et al., *Hole transport layers for organic solar cells: recent progress and prospects*. Journal of Materials Chemistry A, 2020. **8**(23): p. 11478-11492.DOI: 10.1039/d0ta03511d.
- [16]. Rombach, F.M., S.A. Haque, and T.J. Macdonald, *Lessons learned from spiro-OMeTAD and PTAA in perovskite solar cells*. Energy & Environmental Science, 2021. **14**(10): p. 5161-5190.DOI: doi.org/10.1039/D1EE02095A.
- [17]. Cameron, J. and P.J. Skabara, *The damaging effects of the acidity in PEDOT: PSS on semiconductor device performance and solutions based on non-acidic alternatives*. Materials Horizons, 2020. **7**(7): p. 1759-1772.DOI: https://doi.org/10.1039/C9MH01978B.
- [18]. Singh, R., et al., *Review of current progress in inorganic hole-transport materials for perovskite solar cells*. Applied Materials Today, 2019. **14**: p. 175-200.
- [19]. Chen, Y., et al., *SnO₂-based electron transporting layer materials for perovskite solar cells: A review of recent progress*. Journal of energy chemistry, 2019. **35**: p. 144-167.DOI: https://doi.org/10.1016/j.jechem.2018.11.011.
- [20]. Ozgur, U., *A comprehensive review of ZnO materials and devices*. J. Appl. Phys., 2005. **98**(41301): p. 1-103.DOI: https://doi.org/10.1063/1.1992666.
- [21]. Assi, A.A., W.R. Saleh, and E. Mohajerani, *Investigate of TiO₂ and SnO₂ as electron transport layer for perovskite solar cells*, in *The 8th international conference on applied science and technology (ICAST 2020)*. 2020.
- [22]. Zhuang, J., J. Wang, and F. Yan, *Review on chemical stability of lead halide perovskite solar cells*. Nano-Micro Letters, 2023. **15**(1): p. 84.DOI: https://doi.org/10.1007/s40820-023-01046-0.
- [23]. Hossain, M.K., et al., *Effect of various electron and hole transport layers on the performance of CsPbI₃-based perovskite solar cells: A numerical investigation in DFT, SCAPS-1D, and wxAMPS frameworks*. ACS omega, 2022. **7**(47): p. 43210-43230.DOI: doi.org/10.1021/acsomega.2c05912.
- [24]. Idrissi, S., et al., *DFT and TDDFT studies of the new inorganic perovskite CsPbI₃ for solar cell applications*. Chemical Physics Letters, 2021. **766**: p. 138347.DOI: https://doi.org/10.1016/j.cplett.2021.138347.
- [25]. Karthick, S., J. Bouclé, and S. Velumani, *Effect of bismuth iodide (BiI₃) interfacial layer with different HTL's in FAPI based perovskite solar cell-SCAPS-1D study*. Solar Energy, 2021. **218**: p. 157-168.DOI: https://doi.org/10.1016/j.solener.2021.02.041.
- [26]. Pindolia, G., S.M. Shinde, and P.K. Jha, *Optimization of an inorganic lead free RbGeI₃ based perovskite solar cell by SCAPS-1D simulation*. Solar Energy, 2022. **236**: p. 802-821.DOI: https://doi.org/10.1016/j.solener.2022.03.053.
- [27]. Abdelaziz, S., et al., *Investigating the performance of formamidinium tin-based perovskite solar cell by SCAPS device simulation*. Optical Materials, 2020. **101**: p. 109738.DOI: doi.org/10.1016/j.optmat.2020.109738.
- [28]. Stanic, D., et al., *Simulating the Performance of a Formamidinium Based Mixed Cation Lead Halide Perovskite Solar Cell*. Materials (Basel), 2021. **14**(21).DOI: 10.3390/ma14216341.
- [29]. Azri, F., et al., *Electron and hole transport layers optimization by numerical simulation of a perovskite solar cell*. Solar Energy, 2019. **181**: p. 372-378.DOI: 10.1016/j.solener.2019.02.017.
- [30]. Minemoto, T. and M. Murata, *Impact of work function of back contact of perovskite solar cells without hole transport material analyzed by device simulation*. Current Applied Physics, 2014. **14**(11): p. 1428-1433.DOI: 10.1016/j.cap.2014.08.002.
- [31]. Burgelman, M., P. Nollet, and S. Degraeve, *Modelling polycrystalline semiconductor solar cells*. Thin solid films, 2000. **361**: p. 527-532.DOI: https://doi.org/10.1016/S0040-6090(99)00825-1.
- [32]. Houimi, A., et al., *Numerical analysis of CZTS/n-Si solar cells using SCAPS-1D. A comparative study between experimental and calculated outputs*. Optical Materials, 2021. **121**: p. 111544.DOI: https://doi.org/10.1016/j.optmat.2021.111544.
- [33]. Bush, K.A., et al., *23.6%-efficient monolithic perovskite/silicon tandem solar cells with improved stability*. Nature Energy, 2017. **2**(4): p. 1-7.DOI: https://doi.org/10.1038/nenergy.2017.9.
- [34]. Köhnen, E., et al., *Highly efficient monolithic perovskite silicon tandem solar cells: analyzing the influence of current mismatch on device performance*. Sustainable Energy & Fuels, 2019. **3**(8): p. 1995-2005.DOI: doi.org/10.1039/C9SE00120D.
- [35]. Biswal, S.R. and J.P. Kar, *Effect on electrical properties of CuI thin film prepared by a spin coating technique*. Materials Today: Proceedings, 2023. **76**: p. 403-405.DOI: https://doi.org/10.1016/j.matpr.2022.11.504.
- [36]. Kaushik, D.K., et al., *Thermal evaporated Copper Iodide (CuI) thin films: A note on the disorder evaluated through the temperature dependent electrical properties*. Solar Energy Materials and Solar Cells, 2017. **165**: p. 52-58.DOI: https://doi.org/10.1016/j.solmat.2017.02.030.
- [37]. Kim, J., K.S. Kim, and C.W. Myung, *Efficient electron extraction of SnO₂ electron transport layer for lead halide perovskite solar cell*. npj Computational Materials, 2020. **6**(1): p. 100.DOI: https://doi.org/10.1038/s41524-020-00370-y.
- [38]. Chen, J.-Y., et al., *Low-temperature electrodeposited crystalline SnO₂ as an efficient electron-transporting layer for conventional perovskite solar cells*. Solar Energy Materials and Solar Cells, 2017. **164**: p. 47-55.DOI: https://doi.org/10.1016/j.solmat.2017.02.008.
- [39]. Du, H.-J., W.-C. Wang, and J.-Z. Zhu, *Device simulation of lead-free CH₃NH₃SnI₃ perovskite solar cells with high efficiency*. Chinese Physics B, 2016. **25**(10): p. 108802.DOI: 10.1088/1674-1056/25/10/108802.

- [40]. Liu, D. and T.L. Kelly, *Perovskite solar cells with a planar heterojunction structure prepared using room-temperature solution processing techniques*. Nature photonics, 2014. **8**(2): p. 133-138.DOI: <https://doi.org/10.1038/nphoton.2013.342>.
- [41]. Stamate, M.D., *On the dielectric properties of dc magnetron TiO₂ thin films*. Applied Surface Science, 2003. **218**(1-4): p. 318-323.
- [42]. Bansal, S. and P. Aryal. *Evaluation of new materials for electron and hole transport layers in perovskite-based solar cells through SCAPS-1D simulations*. in 2016 IEEE 43rd Photovoltaic Specialists Conference (PVSC). 2016. IEEE.
- [43]. Chouhan, A.S., N.P. Jasti, and S. Avasthi, *Effect of interface defect density on performance of perovskite solar cell: Correlation of simulation and experiment*. Materials Letters, 2018. **221**: p. 150-153.
- [44]. Gan, Y., et al., *Numerical Simulation of High-Performance CsPbI₃/FAPbI₃ Heterojunction Perovskite Solar Cells*. Energies, 2022. **15**(19): p. 7301.
- [45]. Madan, J., et al., *Numerical simulations of PbS colloidal quantum dots solar cell with ZnO: PEIE-based electron transport layer*. Indian Journal of Physics, 2022. **96**(14): p. 4203-4208.DOI: <https://doi.org/10.1007/s12648-022-02354-8>.
- [46]. Pandey, R., et al., *Device simulations: Toward the design of > 13% efficient PbS colloidal quantum dot solar cell*. Solar Energy, 2020. **207**: p. 893-902.DOI: <https://doi.org/10.1016/j.solener.2020.06.099>.
- [47]. Park, S.Y. and K. Zhu, *Advances in SnO(2) for Efficient and Stable n-i-p Perovskite Solar Cells*. Adv Mater, 2022. **34**(27): p. e2110438.DOI: 10.1002/adma.202110438.
- [48]. Ratchagar, V. and K. Jagannathan, *Synthesis and characterization of SnO₂ nano particles for carbon absorbing applications*. Oriental Journal of Chemistry, 2016. **32**(1): p. 207-212.DOI: 10.13005/ojc/320121.
- [49]. Jin, H., et al., *It's a trap! On the nature of localised states and charge trapping in lead halide perovskites*. Materials Horizons, 2020. **7**(2): p. 397-410.DOI: <https://doi.org/10.1039/C9MH00500E>.
- [50]. Guo, Z., et al., *The high open-circuit voltage of perovskite solar cells: a review*. Energy & Environmental Science, 2022. **15**(8): p. 3171-3222.DOI: doi.org/10.1039/D2EE00663D.
- [51]. Rai, S., B. Pandey, and D. Dwivedi, *Modeling of highly efficient and low cost CH₃NH₃Pb (1-x)Cl_x 3 based perovskite solar cell by numerical simulation*. Optical Materials, 2020. **100**: p. 109631.DOI: <https://doi.org/10.1016/j.optmat.2019.109631>.
- [52]. Samiul Islam, M., et al., *Defect study and modelling of SnX₃-based perovskite solar cells with SCAPS-1D*. Nanomaterials, 2021. **11**(5): p. 1218.DOI: <https://doi.org/10.3390/nano11051218>.
- [53]. De Los Santos, I.M., et al., *Optimization of CH₃NH₃PbI₃ perovskite solar cells: A theoretical and experimental study*. Solar Energy, 2020. **199**: p. 198-205.DOI: <https://doi.org/10.1016/j.solener.2020.02.026>.
- [54]. Correa-Baena, J.-P., et al., *Identifying and suppressing interfacial recombination to achieve high open-circuit voltage in perovskite solar cells*. Energy & Environmental Science, 2017. **10**(5): p. 1207-1212.DOI: <https://doi.org/10.1039/C7EE00421D>.
- [55]. Huang, L., et al., *Electron transport layer-free planar perovskite solar cells: further performance enhancement perspective from device simulation*. Solar Energy Materials and Solar Cells, 2016. **157**: p. 1038-1047.DOI: <https://doi.org/10.1016/j.solmat.2016.08.025>.
- [56]. Jannat, F., S. Ahmed, and M.A. Alim, *Performance analysis of cesium formamidinium lead mixed halide based perovskite solar cell with MoO_x as hole transport material via SCAPS-1D*. Optik, 2021. **228**: p. 166202.DOI: <https://doi.org/10.1016/j.ijleo.2020.166202>.
- [57]. Lin, L., et al., *Boosting efficiency up to 25% for HTL-free carbon-based perovskite solar cells by gradient doping using SCAPS simulation*. Solar Energy, 2021. **215**: p. 328-334.DOI: <https://doi.org/10.1016/j.solener.2020.12.059>.