

## Article

# Investigating the Performance of Efficient and Stable Planar Perovskite Solar Cell with an Effective Inorganic Carrier Transport Layer Using SCAPS-1D Simulation

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**Abstract:** Organic–inorganic metal halide perovskite (OIMHP) has emerged as a promising material for solar cell application due to their outstanding optoelectronics properties. The perovskite-based solar cell (PSC) demonstrates a significant enhancement in efficiency of more than 20%, with a certified efficiency rating of 23.13%. Considering both the Shockley limit and bandgap, there exists a substantial potential for further efficiency improvement. However, stability remains a significant obstacle in the commercialization of these devices. Compared to organic carrier transport layers (CTLs), inorganic material such as ZnO, TiO<sub>2</sub>, SnO<sub>2</sub>, and NiO<sub>x</sub> offer the advantage of being deposited using atomic layer deposition (ALD), which in turn improves the efficiency and stability of the device. In this study, methylammonium lead iodide (MAPbI<sub>3</sub>)-based cells with inorganic CTL layers of SnO<sub>2</sub> and NiO<sub>x</sub> are simulated using SCAPS-1D software. The cell structure configuration comprises ITO/SnO<sub>2</sub>/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/NiO<sub>x</sub>/Back contact where SnO<sub>2</sub> and NiO<sub>x</sub> act as ETL and HTL, respectively, while ITO is a transparent front-end electrode. Detailed investigation is carried out into the influence of various factors, including MAPbI<sub>3</sub> layer size, the thickness of CTLs, operating temperature parasitic resistance, light intensity, bulk defects, and interfacial defects on the performance parameters. We found that the defects in layers and interface junctions greatly influence the performance parameter of the cell, which is eliminated through an ALD deposition approach. The optimum size of the MAPbI<sub>3</sub> layer and CTL was found to be 400 nm and 50 nm, respectively. At the optimized configuration, the PSC demonstrates an efficiency of 22.13%, short circuit current (JSC) of 20.93 mA/m<sup>2</sup>, open circuit voltage (V<sub>OC</sub>) of 1.32 V, and fill factor (FF) of 70.86%.

**Keywords:** perovskite solar cell; inorganic CTLs; SCAPS-1D; stability



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## 1. Introduction

The PSC has recently received a lot of attention due to a significant increase in power conversion efficiency (PCE) and advancements in design and manufacturing techniques [1]. According to the NREL cell efficiency chart, the efficiency of PSC has reached 26%. In the last six years, PSC efficiency has increased by 2.27% per year from the first developed PSC of 9.7%, which has greatly surpassed other kinds of solar cells, which have increased by less than 1.0% per year [2]. PCE advancements were made possible by scientific knowledge as well as engineering advancements. The former refers to the crystal formation, composition alteration, and optoelectronics capabilities, while the latter refers to interfacial changing and the formation of highly efficient carrier transportation layers (CTLs). CTLs are subdivided into electron and hole transport layers (ETLs and HTLs) [2].

The fundamental design of PSC consists of perovskite material sandwiched between the ETL and HTL in NIP or PIN configuration. Under solar illumination, the light interacts with a PSC structure from the upper side through the glass substrate coated with transparent electrodes such as tin-doped indium oxide, HTL, or ETL, which is finally absorbed by the perovskite layer and photo-generated electron-hole pairs are created. In this process, there are several possibilities for the incident photon, for example, the photon might be reflected or scattered and will not contribute to the photo-current of the PSC [3]. One strategy is to apply an antireflection coating to reduce photon losses on the glass substrate. However, it will eventually increase the PSC production cost [4].

The ETL transport electron, utilizing n-type material and its conduction band minimum (CBM), should be smaller than the perovskite material. The HTL requires p-type materials with a higher valence band maximum (VBM) than the perovskite material.

The main obstacles in commercializing PSCs are their stability (life span). They are more sensitive to external stimuli such as light, heat, oxygen, and water. PSCs exposed to such conditions can cause rapid degradation of the cell structure that in turn causes cell failure, leaving harmful effect on the biological environment by releasing toxic elements such as Pb ions [5].

The performance is further reduced because of the inappropriate selection of ETLs and HTLs. Most commonly used PSCs in NIP configurations use  $\text{TiO}_2$  as the ETL, while Spiro-OMeTAD is employed as the HTL and in PIN, PEDOT: PSS, and PTAA are used as HTL.  $\text{TiO}_2$  shows poor stability against ultraviolet (UV) radiation and needs additional layers to screen the UV rays. Spiro-OMeTAD shows inadequate thermal and air stability, while PEDOT: PSS did not sustain its stability for a long time due to its acidic and hygroscopic properties [6–8].

Compared to organic, inorganic CTL-based PSCs have been recently developed which display excellent properties. Some inorganic material used for ETLs include  $\text{SnO}_2$ ,  $\text{TiO}_2$ ,  $\text{ZnO}$ ,  $\text{BaSnO}_3$ , and  $\text{Zn}_2\text{SnO}_4$ , and those used for HTL include  $\text{NiO}_x$ ,  $\text{CuI}$ ,  $\text{MoO}_3$ ,  $\text{CrO}_x$ , and  $\text{CuO}_x$  [2].

Another significant factor that enhanced the efficiency and stability of PSC is the deposition technique. Compare to other deposition techniques, ALD is an excellent tool to deposit defect-free thin-films with higher accuracy and conformity. The PSC fabrication, which includes the deposition of ETL and HTL layers, passivation or interference layers, and encapsulation of the device can be easily achieved with ALD tools, and can be considered an upgrade in cell performance [2,9,10]. It is important to decrease the series resistances and increase the shunt resistance, which is associated with the thickness and quality of the CTLs and perovskite layers [11]. The ordinary thin-films containing cracks and pinholes that provide pathways to shunt leakage current that can badly affect the cell's performance. In contrast, thickening CTL layers can increase the series resistance, which drops the output voltage [12,13]. In this scenario, ALDs can provide an excellent CTL layer, having uniform and dense film formation along with accurate control in the sub-nanometer range.

Similarly, in PSC, the interference between perovskite and CTL layers are the main source of electron-hole recombination (losses) which directly affect the efficiency of PV cells. The surface passivation technique is used to deposit ultra-thin layer at low temperatures at the surface to avoid thermally generated cracks and pinholes in the layers [14]. ALDs have been widely adopted as a solution in the P.V. industry to provide high-quality, low-temperature, and uniform passivation layers. With the help of the passivation layer, it not only improves cell efficiency, but also increases the stability of PSCs by protecting them from environmental hazard conditions.

Numerical simulation is the best theoretical approach to predict the solar cell performance before developing a prototype. SCAPS-1D is widely utilized in research on solar cells, including PSC, to examine the performance parameters. Hossain et al. [15] simulated lead-free  $\text{Sc}_3\text{Bi}_2\text{I}_9$ -based PSCs using SCAPS for 49 different configurations, and found that  $\text{Cu}_2\text{O}$  is a cost-effective and efficient HTL layer for lead-free PSC. Saha et al. [16] simulated (SCAPS-1D)  $\text{MaPbI}_3$ -based PSCs with graphene-doped  $\text{TiO}_2$  ETLs and PTAA

as HTLs recorded an efficiency of 22.7%. Mushtaq et al. [17] developed PSC having a configuration FTO/SnO<sub>2</sub>/MASnBr<sub>3</sub>/NiO/Au demonstrating the potential of MASnBr<sub>3</sub>, an eco-economical, high-performance, and removable energy solution. Hussain et al. [18] investigated lead-free CH<sub>3</sub>NH<sub>3</sub>SnI<sub>3</sub> with SnO<sub>2</sub> and Spiro-OMeTAD recorded an efficiency of 33.26%. Sunny et al. [19] developed a SCAPS model of HTL-free PSCs using CH<sub>3</sub>NH<sub>3</sub>SnI<sub>3</sub> and TiO<sub>2</sub> ETL and the optimized structure achieved a 6.33% efficiency, making it a cost-effective and efficient PSC. Ibrahim et al. [20] investigated the effect defect in the absorber and ETL/perovskite interference of PSCs using SCAPS tool. The result shows that varying defect density from 10<sup>10</sup> cm<sup>−3</sup> to 10<sup>18</sup> cm<sup>−3</sup> causes significant drops in the performance parameter of the cell. Samiul Islam et al. [21] study lead-free CH<sub>3</sub>NH<sub>3</sub>SnBr<sub>3</sub>-based PSCs. The model explores the effects of defects, parasitic resistance, and work functions of the contact. Similarly, Basyoni et al. [22] investigated interference defects between CTLs with lead- and lead-free PSCs to optimize the performance using a SCAPS simulator. It reveals that defects play a crucial role in increasing the efficiency of lead-free PSCs from 1.76% to 5.35%, highlighting the importance of interface engineering in PSC design. In this study, we will explore the performance of PSCs using inorganic CTL materials that can be easily deposited with ALD, such as ZnO, TiO<sub>2</sub>, SnO<sub>2</sub>, and NiO<sub>x</sub>, utilizing the SCAPS tool. These materials have the benefit of being deposited using ALD processes, which improves the device's efficiency and stability.

The NiO<sub>x</sub> is a favorable HTL material used for several photovoltaic (P.V) application due to its intrinsic p-type semiconductor nature, superior hole extraction property, low processing temperature, good optical properties, low-cost, and good chemical and thermal stability [23–25].

Similarly, SnO<sub>2</sub>-based PSC efficiency is recorded up to 25%, making SnO<sub>2</sub> to be a good ETL choice in PSCs, and a potential substitute for TiO<sub>2</sub> [26,27]. The SnO<sub>2</sub> has extraordinary properties which are required for efficient and stable PSCs, including high-bulk electron mobility and conductivity [28,29], high temperature flexible deposition, large bandgap (3.6–4.5 eV), high optical transparency, and excellent stability under heat, moisture, and light with negligible photo-activity [30,31]. Compared to TiO<sub>2</sub>, SnO<sub>2</sub> ETL requires less temperature (<200 °C) when using chemical bath deposition or spin coating, which is an advantage when it comes to mass production. However, there are certain flaws in the hetero interference that degrade the performance of PSCs due to the mismanagement of the perovskite film and metal oxide. Therefore, the passivation layer of Al<sub>2</sub>O<sub>3</sub> on the SnO<sub>2</sub> layer is used to upgrade the performance of SnO<sub>2</sub>-based PSCs [32]. In addition to this, NiO<sub>x</sub> and SnO<sub>2</sub> material show negligible hysteresis behaviors that will help to disclose the actual performance of the PSC.

## 2. SCAPS Simulation

The numerical simulation is the best and easiest approach to comprehend the fundamental operation of the solar cell, revealing the factors that influence their functionality. This investigation was carried out with the help of the SCAPS-1D (solar cell capacitance simulator) software application. SCAPS-1D was developed by Marc Burgelman at the University of Gent, solving thin-film structures in one dimension using electrical and optical parameters [33]. This simulation tool utilizes well-known semiconductor equations such as Poisson's equation, continuity equation, and transport equation to solve the solar cell model and provide parameter measurements of the designed PV cell. The Poisson's equation is used to obtain internal potential distribution within the cell. The continuity equation describes the rate of change in the concentration of carriers (electrons and holes). The transport equation provides information of how the electrons and hole travels in the cell structure. Once the cell structure is defined, the SCAPS solve the following equation from (1)–(5) providing the performance capability of the device.

$$\frac{\partial^2}{\partial x^2} \varphi(x) = \frac{q}{\epsilon} [n(x) - p(x)] \quad (1)$$

$$\frac{\partial n,p}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + (G_x - R_n) + \frac{1}{q} \frac{\partial J_p}{\partial x} + (G_x - R_p) \quad (2)$$

$$J_{n,p} = q\mu_n nE + qD_n \frac{\partial n}{\partial x} + q\mu_p pE + qD_p \frac{\partial p}{\partial x} \quad (3)$$

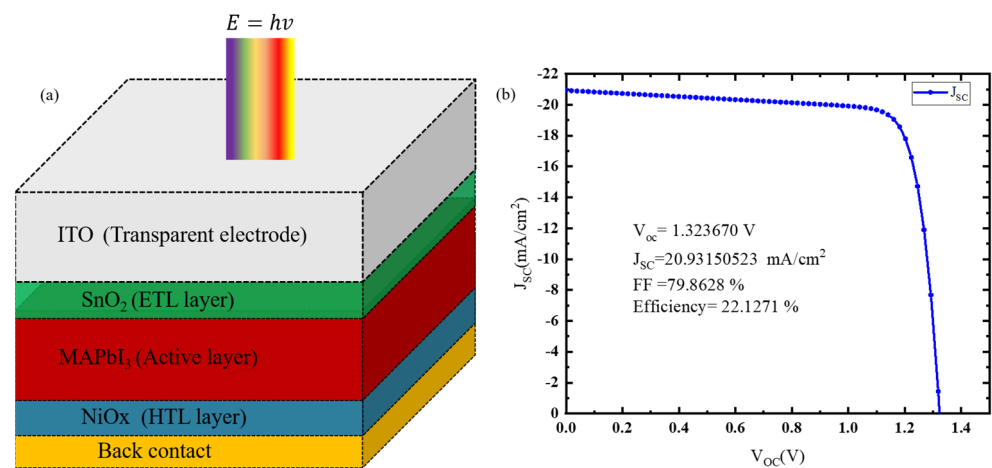
$$D_{n,p} = \left( \frac{K_b T}{q} \right) \mu_{n,p} \text{ and } L_{n,p} = \sqrt{D\tau} \quad (4)$$

$$V_{OC} = V_T \ln \left\{ \left( \frac{I_{light}}{I_0} \right) + 1 \right\} \quad (5)$$

where  $\epsilon$  is permittivity,  $q$  is the elementary charge,  $\varphi(x)$  stands for electrostatic potential,  $n$  and  $p$  are electron and hole density,  $E$  is the electric field,  $D_n$  and  $D_p$  are the diffusion coefficient, and  $\mu_n$  and  $\mu_p$  are carriers' mobility. The expression of diffusivity in Equation (4) refers to the ability of carriers to scatter or spread out within the materials where the diffusion length  $L_{n,p}$  indicates the distance traveled by the carriers between the generation and recombination period. When no external load is applied, the terminal voltage is considered open circuit voltage ( $V_{OC}$ ) given by Equation (5). Similarly, when the terminal of the solar cell is short circuited with each other, ( $V_{OC}$  become zero) it provides a reading of the short circuit current or the light-generated current.

### 3. Proposed Device Model

The proposed Perovskite solar cell (PSC) layer configuration is shown in Figure 1a. The various electrical parameters of the material used in PSC simulation are shown in Table 1, while Table 2 display parameters taken for interface defects. The framework of the cell consists of ITO/SnO<sub>2</sub>/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/NiO<sub>x</sub>/Back contact. The transparent electrode ITO serves two functions: anode collecting electron for an external load and passing light spectrum to the internal cell structure. SnO<sub>2</sub> act as the ETL, which passes electrons easily while blocking the holes. The methylammonium lead iodide (CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>) is a light-absorbing layer where electron-hole pairs are created under illumination. NiO<sub>x</sub> acts as the hole transport layer medium while blocking the electron. The overall device exhibits NIP configuration in which SnO<sub>2</sub> is an n-type material, CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> as an intrinsic semiconductor, and NiO<sub>x</sub> is a p-type material. The selection of CTL materials in PSC design is crucial for the device's performance, as efficient CTL layers provide higher conductivity and reduce recombination losses of carriers. The material used for the ETL typically has a LUMO (lowest un-occupied molecular orbital) energy lower than or equal to the LUMO energy of the active layer. The natural tendency of electrons to move from high to low energy levels facilitates electron transport while hindering the movement of holes. Similarly, HTL material should have a HOMO (highest occupied molecular orbital) energy equal to or higher than that of the active material. Holes always tend to move from low to higher energy levels. This mechanism ensures efficient hole transport while blocking electrons. The band alignment diagram of our proposed device is shown in Figure S1. All the simulations were performed at a standard test temperature of 300 K and a standard test illumination condition of 100 w/m<sup>2</sup>. The series and shunt resistance are considered 1  $\Omega \cdot \text{cm}^2$  and  $1.0 \times 10^3 \Omega \cdot \text{cm}^2$ , respectively. The optimum thickness of the PSC was founded 300 nm/50 nm/400 nm/50 nm at which the cell recorded an efficiency of around 22.1%. In addition, the proper thickness of the CTL is required to avoid the short circuit effect in the cell structure due to sputtering damage.



**Figure 1.** (a) Proposed PSC layer configuration; (b) optimum J-V curve.

**Table 1.** Material parameter used for simulation.

Parameters	Materials			
	ITO [34]	NiO <sub>x</sub>	CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub>	SnO <sub>2</sub>
Thickness (nm)	300	50–200	100–1600	50–200
Dielectric constant	9.00	10.7 [35]	10.0 [35]	8.00 [35]
Electron affinity ( $\chi$ (eV))	4.00	2.1 [36]	4.1 [37]	3.93 [38]
Bandgap, $E_g$ (eV)	3.5	3.7 [39]	1.6 [40,41]	3.6 [38]
Effective conduction band density, $N_c$ (cm <sup>-3</sup> )	$2.2 \times 10^{18}$	$2.8 \times 10^{19}$ [42]	$2 \times 10^{18}$	$3.1 \times 10^{18}$ [43]
Effective valence band density, $N_v$ (cm <sup>-3</sup> )	$1.8 \times 10^{19}$	$1.8 \times 10^{19}$ [42]	$1 \times 10^{18}$	$2.5 \times 10^{19}$ [43]
Mobility of electron, $\mu_n$ (cm <sup>2</sup> /(V s))	20	12.0 [44]	100	15 [45]
Mobility of hole, $\mu_p$ (cm <sup>2</sup> /(V s))	10	25.0 [44]	100	0.1 [45]
Donor concentration ND (cm <sup>-3</sup> )	$1.0 \times 10^{21}$	0.0	$1 \times 10^9$	$10^{19}$
Acceptor concentration NA (cm <sup>-3</sup> )	0	$1 \times 10^{15}$	$1 \times 10^9$	0.0
Defect density (1/cm <sup>3</sup> )	$1 \times 10^{15}$	$1 \times 10^{14}$	$1 \times 10^{14}$	$1 \times 10^{14}$
Absorption coefficients ( $\alpha$ )	[46]	[47]	[47]	[47]

**Table 2.** Parameter used for interface defects [48].

Parameters	ETL/MAPbI <sub>3</sub>	HTL/MAPbI <sub>3</sub>
Defect type	Neutral	Neutral
Capture cross section of electrons (cm <sup>-2</sup> )	$1 \times 10^{19}$	$1 \times 10^{19}$
Capture cross section of holes (cm <sup>-2</sup> )	$1 \times 10^{-19}$	$1 \times 10^{19}$
Energetic distribution	Single	Single
Reference for defect energy level Et	Above the highest EV	Above the highest EV
Reference energy (eV)	0.6	0.6
Total density (1/cm <sup>2</sup> )	$1 \times 10^{10}$ – $1 \times 10^{20}$	$1 \times 10^{10}$ – $1 \times 10^{20}$

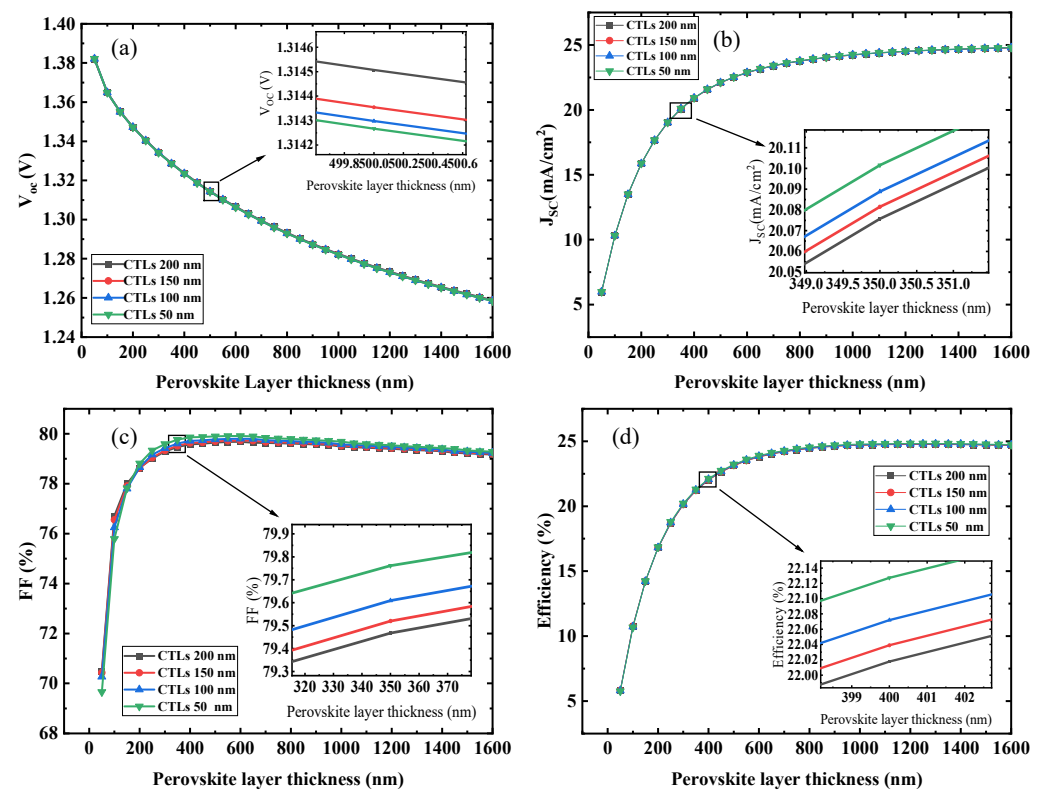
## 4. Result and Discussion

### 4.1. Effects of Layer Thickness

The thickness of the active or photon-absorbing layer (MAPbI<sub>3</sub>) has significant impacts on the PSC's performance. A very thin absorbing layer harvesting a small portion of the photons create a smaller number of electron-hole pairs which directly reduce the efficiency of the solar cell. In contrast, a very thick absorber layer lowers the cell's efficiency due to recombination losses [49,50]. Thus, it is essential to find the optimum thickness of MAPbI<sub>3</sub>. To determine the optimum thickness of the perovskite material layer, the thickness of the MAPbI<sub>3</sub> is varied from 100 nm to 1600 nm, while in parallel, the thickness of the CTL layer is from 50 nm to 200 nm in four steps. The cell is simulated under standard test conditions (STCs) of 1000 W/m<sup>2</sup> (A.M 1.5 G) and a standard test temperature (STT) of



300 K. The cell performance parameter such as  $V_{OC}$ ,  $\eta$ , FF, and  $J_{SC}$  in response to layer thickness is shown in Figure 2. We observed  $V_{OC}$  (Figure 2a) is directly affected by the increase in thickness due to the increase in parasitic resistance. The FF increases from 100 to 400 nm and then starts to decrease, which is also caused by the parasitic resistance. The increase in thickness ensures a larger area for photon absorption and hence a high number of electron-hole pairs resulting in high efficiency, above 400 nm the efficiency is slowly increased because of the low extraction rate of the carriers. The fundamental cause of the cell efficiency improvement with the thickness is due to the increase in optical density. However, when the diffusion length of the carrier is less than the active layer thickness, the carriers will recombine before crossing the CTL layer [23]. The other parameters,  $J_{SC}$  and cell efficiency, increase logarithmically; at 400 nm MAPbI<sub>3</sub> and 50 nm CTL thickness, the PSC efficiency reached 22.13%. It may be deduced that an increase in thickness beyond 400 nm can reduce the FF of the PSC. In addition to this, insubstantial improvements in efficiency come at the expense of material quantity, which is economically unacceptable. The optimal layer thicknesses for MAPbI<sub>3</sub> and CTL are 400 nm and 50 nm, respectively. The J–V curve and the performance parameter of the cell at the optimum size is shown in Figure 1b.

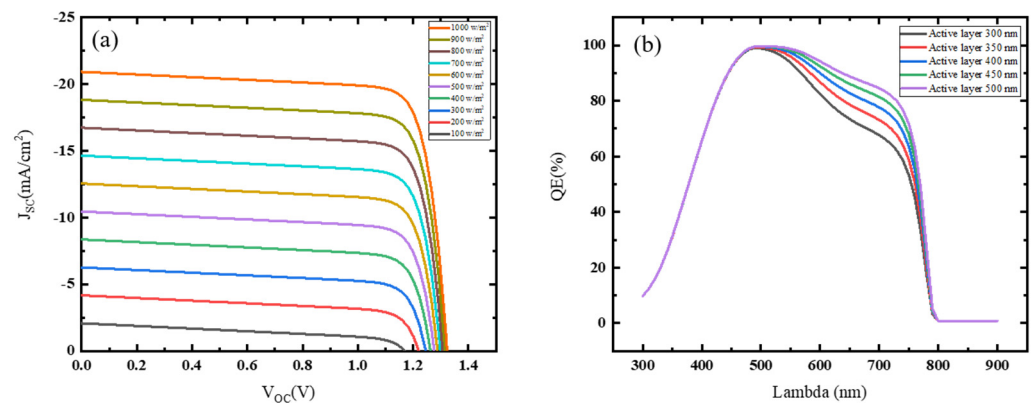


**Figure 2.** Optimization of MAPbI<sub>3</sub> and CTLs layer thickness on solar cell parameters: (a) Open-circuit voltage (b) Short-circuit current density (c) Fill factor (d) Efficiency.

#### 4.2. Effects of Light Intensity and Quantum Efficiency

The primary input source of energy that activates the solar cell is sunlight, and the intensity of the sunlight is not fixed and varies from 0 to 1 kW/m<sup>2</sup> due to the continuous changing of the sun's position. This illumination fluctuation greatly affects the solar cell's performance [51]. To counter this problem, a solar tracking mechanism is introduced that allows solar module to track the sun's daily passage from east to west or MPPT electrical device that manipulate the electrical parameter (voltage or current) to ensure high power is obtained from the solar cell [52]. The solar cell integrated with such an intriguing gadget offers continuous peak power throughout the daytime. AM1.5 G or 1 kW/m<sup>2</sup> (equal to one sun) is a STC at which a commercial solar cell performance is measure before finalizing

the product. Similarly, the value of  $10 \text{ kw/m}^2$  indicates that the cell is exposed to 10 suns. Although the number of 10 suns is technically impossible, it is indirectly employed for concentrated solar cells. The designed PSC is also tested under such circumstances. The light intensity is varied from  $100 \text{ w/m}^2$  to  $1000 \text{ w/m}^2$  at STC of 300 K. The J–V curve of the PSC's various illumination intensities are shown in Figure 3a. We noticed that  $V_{OC}$  and  $J_{SC}$  are directly proportional to the intensity of light, which directly affects the output power and efficiency of the solar cell.



**Figure 3.** (a) Impact of light intensity on  $V_{OC}$  and  $J_{SC}$ ; (b) quantum efficiency in response to wave-length.

Similarly, quantum efficiency (QE) of the PV cell can be described by the ratio of the numbers of carrier captured by the cell to the incident number of photons of a given energy. It specifies how the device reacts to the various illumination wavelengths [53]. When photons of a given energy or wavelength are absorbed and the resultant minority's carrier are accumulated, the QE is said to be at unity with that wavelength. QEs with different active layer thicknesses are shown in Figure 3b. QE as a function of lambda is investigated within the range of 300 nm to 900 nm. The QE rise from 300 nm to 800 nm, and the highest peak is observed between 450 nm to 550 nm, following the reduction in the QE and reaching zero. The square shape of the QE curve (ideal condition) is also affected by the active layer thickness of the solar cell, which is observed.

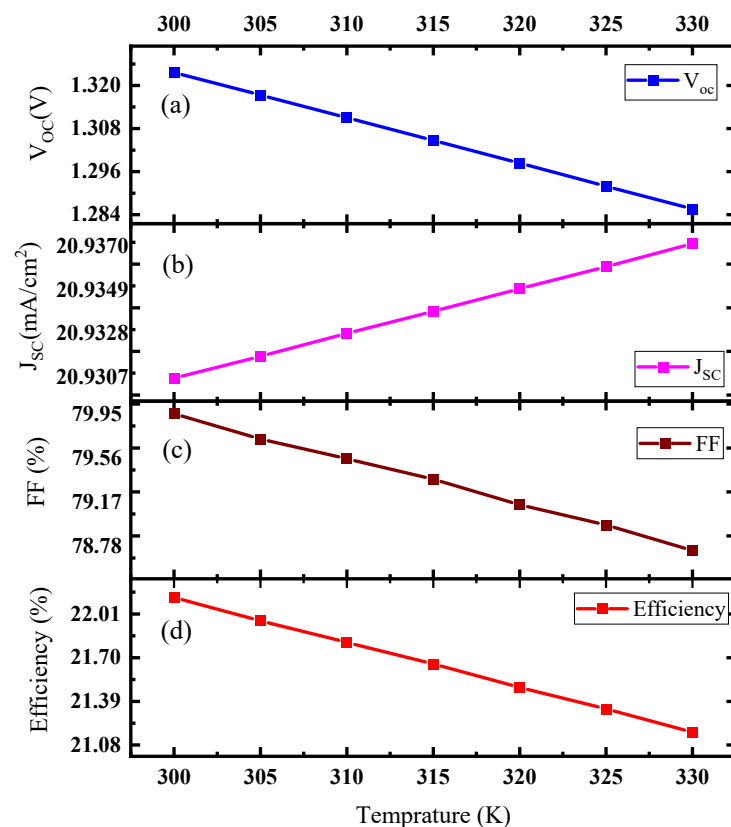
#### 4.3. Effects of Temperature

The PSC performance is substantially affected by the operating temperature. Generally, STT 300 K is employed for simulation purposes. However, in natural environments, this number is not constant and changes over the year. High temperatures cause deformations in the cell structure, introducing interfacial defects between the composite layers of the cell [54]. These defects limit the interconnectivity of the PSC layer, resulting in a higher rate of recombination and a rise of parasitic resistance ( $R_s$ ) which decrease the PSC efficiency. Higher temperatures also affect electron-hole concentration, carrier mobility, and semiconductor bandgap [55]. The atomic vibration of the semiconductor is sensitive to the temperature. The increase in temperature speeds up atomic vibrations in the semiconductor, which causes an increase in inter-atomic separation. The linear temperature coefficient of a material is used to quantify this effect. As the interatomic space increases, the average electric potential perceived by the electron decreases, eliminating the bandgap size. The interatomic distance can also be changed by applying mechanical stress, resulting in a decrease or increase in the bandgap of the material. Vershni's relation states that the bandgap of a material is temperature dependent and is given by

$$E_{g(T)} = E_{g(0)} - \frac{\alpha T^2}{\beta + T} \quad (6)$$

where  $T$  is the temperature, and  $E_{g(0)}$  (bandgap at 0 K),  $\beta$ , and  $\alpha$  are the material constants. In this simulation, we varied the temperature from 300 K to 330 K while keeping light inten-

sity, parasitic resistance, and thickness of the layers constant. The influence of temperature on the solar cell's performance, as illustrated in Figure 4, is of significance. At an operating temperature of 300 K, the  $V_{OC}$  and FF measures at 1.323 V and 79.86%, respectively. However, as the temperature increases, there is a corresponding decrease in both  $V_{OC}$  and FF, as depicted in Figure 4a,c, eventually resulting in values of 1.285 V and 78.65%, respectively. The  $J_{SC}$  remains relatively constant around 20.93 mA/m<sup>2</sup> (see Figure 4b). However, there is a slight increase from 0.0007 mA/m<sup>2</sup> to 0.0070 mA/m<sup>2</sup> due to the contribution of thermally generated carriers in addition to the light-generated carriers. The  $V_{OC}$  and FF are directly influenced by the adverse effects of temperature, which consequently impacts the overall efficiency of the solar cell. Figure 4d illustrates a decline in efficiency from 22.12% to 21.17%, underscoring the temperature's detrimental impact.



**Figure 4.** Effect of temperature on PSC performance parameter: (a) Open-circuit voltage (b) Short-circuit current density (c) Fill factor (d) Efficiency.

#### 4.4. Effects of Bulk Defects and Interface Defects Density

SCAPS-1D uses the thermionic emission model (TEM) to explore heterojunction layers. Interface defects are analyzed in the same way as bulk defects, and a recombination in these states is assessed by an extension of the SRH theory known as the Pauwels–Vanhoutte theory [56]. These traps facilitate recombination losses, enhancing dark current and hence lowering efficiency. The carrier capture cross-section, energy level, and trap density are basic physical properties that determine how a certain trap impacts the non-radiative recombination rate. The carrier capture cross-section is mostly determined by the material's dielectric constant, while trap density can be technically controlled by eliminating crystallographic defects such as surface and grain boundary imperfections throughout the fabrication process [57].

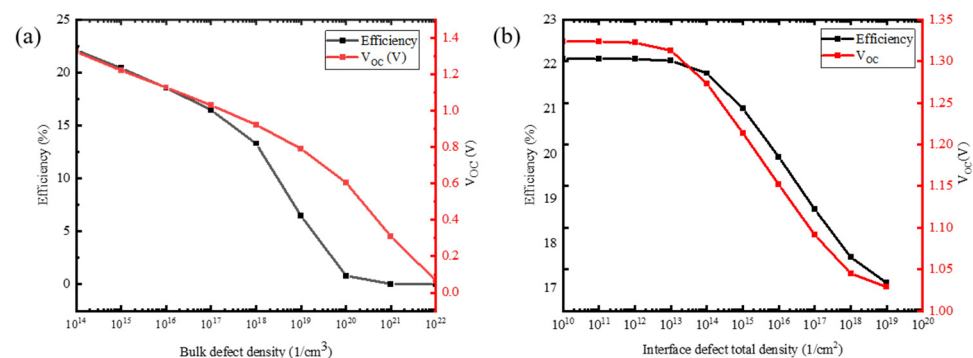
Elementary and neutral vacancy pair defects do not generate deep energy levels within the bandgap; only shallow traps are likely produced, which are not expected to act as potent recombination centers [57]. Furthermore, some contaminants in the PbI<sub>2</sub> reactant, as well as Au residues absorbed in the active layer due to contact deposition, greatly affect the



performance of the cell [58]. To prevent such defects that may result in deep traps, precise manufacturing techniques are required.

PSCs consist of different thin-film materials which are arranged in a sandwich-like structure. Poor deposition of thin-films leaves defects in the materials which greatly affect the performance of the cell [59]. Especially perovskite material exhibits distinct characteristics regarding longer diffusion lengths for electrons and holes ( $L_n$  and  $L_p$ ) in a single crystal. However, this diffusion length significantly fluctuates in thin-film materials, depending upon the quality of the film [35]. In order to examine the impact of defects densities, we introduce defects ranging from  $1 \times 10^{14}$  to  $1 \times 10^{22} \text{ cm}^{-3}$  in all layers of the PSC, including ETLs, HTLs, and perovskite layers.

Figure S2 shows variation in performance parameters such as  $J_{SC}$ ,  $V_{OC}$ , FF, and efficiency follow the expected trend, with a visible reduction as the quality of the layer deteriorates (or defects density increase in thin-films). The  $V_{OC}$  and  $J_{SC}$  decrease from 1.313 V to 0.057 V and 20.77 to 0.06  $\text{mA}/\text{cm}^2$ , respectively. Similarly, FF and efficiency decrease from 79.55% to 24.96% and 22.03 to 0.72%, correspondingly, because of leakage current and parasitic resistance, the light-generated power is dissipated in the cell structure. The defects density of  $1 \times 10^{14}$  has a negligible impact, while above  $1 \times 10^{18}$ , an abrupt decrease is noticed in the cell performance parameters. Defect concentrations in the range of  $1 \times 10^{14}$  to  $1 \times 10^{17}$  are considered acceptable for practical application. In our simulation, we chose a defect density of  $1 \times 10^{14}$ , at which the efficiency and  $V_{OC}$  of the cell is recorded 22.13% and 1.33 V, respectively. The impact of bulk defects on  $V_{OC}$  efficiency are combinedly displayed in Figure 5a.



**Figure 5.** Effects of defects density: (a) bulk defects density; (b) interface defects density.

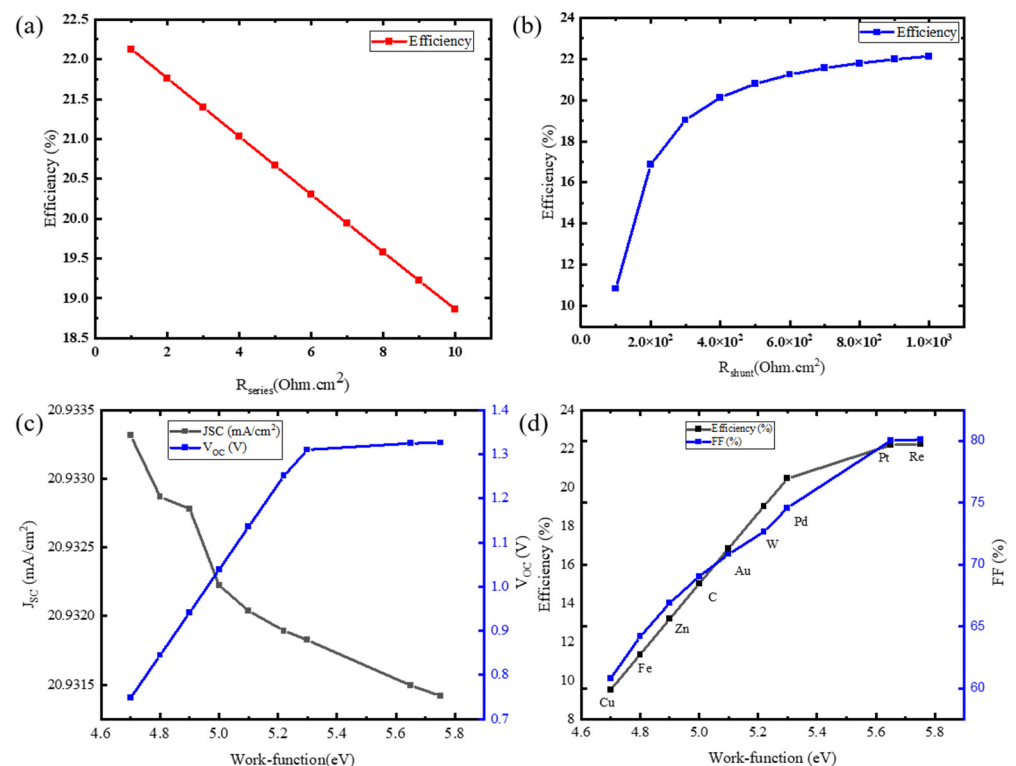
The junction quality plays a crucial role in the device's performance. The presence of defects at the interface increases the recombination rate, resulting in inefficient performance [59,60]. Modeling recombination at the interface is a complex task, and the ideal approach is to introduce a thin defective layer between the junctions to study the effect of the defect at the interface. Here are two thin defective interface layers (DILs) at both sides of the perovskite material layer. The configuration of the cell becomes HTL/DIL/MAPbI<sub>3</sub>/DIL/ETL. The defect density is varied from  $10^{10} \text{ cm}^{-2}$  to  $10^{20} \text{ cm}^{-2}$ . Figure 5b shows the parameter  $V_{OC}$  and efficiency decrease with the increase in defect density at the interface. The DILs inserted between the HTL/MAPbI<sub>3</sub> junction, ETL/MAPbI<sub>3</sub> junction, or placed at both sides of the active layer give the same simulation results. However, the actual performance of the device will be disclosed upon the device fabrication and testing.

#### 4.5. Effects of Parasitic Resistance and Work Function of Back Contact

Resistive effects within solar cells lead to a significant decrease in their efficiency. Some percentage of the light-generated power is dissipated in the cell structure due to these internal resistances. Series and shunt resistances ( $R_S$  and  $R_{SH}$ ) are the two primary types of parasitic resistances ( $R_P$ ) [12,13]. The primary factors responsible for series resistance ( $R_S$ ) comprise the semiconductor material's bulk resistance, interconnection of composite

material layers between each other, metal/semiconductor ohmic contact, and the resistance of the electrode's materials. The shunt resistance is due to the manufacturing defects in the solar cell structure which dissipate a significant amount of light power. Low  $R_{SH}$  provides an alternate path to the carriers' resulting loss of power and lowers the overall efficiency of the device [13]. The researcher tries to keep  $R_S$  and  $R_{SH}$  values at minimum and maximum values, respectively, for optimum design.

We investigated various  $R_P$  values and their impacts on solar cell performance. We noticed that increasing  $R_S$  from 1 to  $10 \Omega \cdot \text{cm}^2$  has no effect on  $V_{OC}$  and minimal influence on  $J_{SC}$ . Other solar cell metrics such as efficiency and FF are constantly dropping with the increase in series resistance (see Figure S3). Similarly, the  $R_{SH}$  is varied from  $0.1 \times 10^3$  to  $1.0 \times 10^3 \Omega \cdot \text{cm}^2$  (see Figure S4), which shows that  $V_{OC}$ , FF,  $J_{SC}$ , and efficiency are improving. The corresponding graph pattern of various parameters shows a significant rise with the increase in shunt resistance. A sharp rise up to  $0.4 \times 10^3$  is visible, followed by a gradual gain with each further increment in  $R_{SH}$ . In our simulation, the values for  $R_S$  and  $R_{SH}$  are considered  $1 \Omega \cdot \text{cm}^2$  and  $1.0 \times 10^3 \Omega \cdot \text{cm}^2$ , respectively, at which point the efficiency reached 22.13% (Figure 6a,b).



**Figure 6.** (a) Influence of shunt resistance on efficiency; (b) efficiency of PSC increases with the increase in shunt resistance; (c) impact of work function on  $V_{OC}$  and  $J_{SC}$ ; (d) impact of work function on FF and efficiency.

The work function and material of the back electrode have a considerable impact on built-in voltage ( $V_{bi}$ ) of a PV cell, resulting in an increase in  $R_S$  of the cell and a decrease in efficiency [61]. A number of materials with different work functions are investigated for the backend electrode to see how they affect the solar cell characteristics, while keeping the front transparent electrode constant. Various materials with different work functions were investigated, including Cu, Fe, Zn, C, Au, W, Pd, Pt, and Re [61–63], to determine how the work function influences solar cell performance. The impact of various materials and their associated work functions on  $J_{SC}$  and  $V_{OC}$  is depicted in Figure 6c. This shows that the work function has little effect on  $J_{SC}$  but a substantial impact on  $V_{OC}$ . Similarly, as the work function increases from 4.7 eV to 5.65 eV, efficiency and FF (Figure 6d) improve significantly.

This enhancement is due to a reduction in the Schottky barrier height between the anode and the HTL, which allows holes to travel more easily from the HTL to the backside of the electrode. Although gold has a reasonable work function for simulation, silver and aluminum are more cost-effective options for the experimentation and commercialization of the solar cell.

## 5. Conclusions

In this research, MAPbI<sub>3</sub>-based PSCs were arranged in NIP configurations of ITO/SnO<sub>2</sub>/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/NiO<sub>x</sub>/Back contact and simulated under standard test conditions of 300 K and A.M 1.5 G. The primary goal is to investigate PSCs with inorganic CTL layers that are easily deposited through the ALD method in order to enhance the efficiency and stability of the cell. We optimized the device using a comprehensive layer-by-layer methodology, including a MAPbI<sub>3</sub> and CTL layer. The optimum thickness of the active and CTL layer was found to be 400 nm and 50 nm, respectively, while taking the bulk defect density of  $1 \times 10^{14} \text{ cm}^{-3}$  in all layers as a constant. In this arrangement, the PSC obtained showed an efficiency of 22.13%, V<sub>OC</sub> of 1.32, J<sub>SC</sub> of 20.93 mA/m<sup>2</sup>, and FF of 79.89%. We also introduced interface defects ( $10^{10} \text{ cm}^{-2}$  to  $10^{20} \text{ cm}^{-2}$ ) between the CTL and perovskite layer; the increase in interface defects can cause poor efficiency of the device which can be eliminated with ALD deposition. Similarly, the influence of parasitic resistance indicates the significance of small R<sub>S</sub> and high values of R<sub>SH</sub>. The design cell's R<sub>S</sub> and R<sub>SH</sub> values are taken to be 1.0 Ω.cm<sup>2</sup> and  $1.0 \times 10^3 \text{ Ω.cm}^2$ , respectively. The work function of ITO is set constant of 4.13 eV, while the different materials have different work functions being tested for back contact at 5.65 eV, and the PSC shows the highest efficiency of 22.13%. In addition, cell parameters are also examined under various practical operating conditions, such as the impact of temperature and light intensity. The design cell's possible parameter aspects are numerically tested and analyzed; however, it is necessary to disclose the stability of the cell structure's with ALD fabrication.

**Supplementary Materials:** The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/en16217438/s1>, Figure S1: PSC band alignment diagram; Figure S2: Effect of bulk defects in the cell structure; Figure S3: Effect of series resistance; Figure S4: Effect of shunt resistance.

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