



# Article Investigation of Electron Transport Material-Free Perovskite/CIGS Tandem Solar Cell

Mostafa M. Salah <sup>1,\*</sup>, Abdelhalim Zekry <sup>2</sup>, Ahmed Shaker <sup>2</sup>, Mohamed Abouelatta <sup>2</sup>, Mohamed Mousa <sup>1</sup> and Ahmed Saeed <sup>1</sup>

- <sup>1</sup> Electrical Engineering Department, Future University in Egypt, Cairo 11835, Egypt
- <sup>2</sup> Faculty of Engineering, Ain Shams University, Cairo 11535, Egypt

\* Correspondence: mostafa.abdulkhalek@fue.edu.eg

**Abstract:** Tandem solar cells have a superb potential to push the power conversion efficiency (PCE) of photovoltaic technologies. They can be also more stable and economical. In this simulation work, an efficient perovskite solar cell (PSC) with Spiro-OMeTAD as a hole transport material (HTM) and with no electron transport material (ETM) to replace the traditional PSC structure is presented. This PSC is then used as a top sub cell together with a copper indium gallium sulfide (CIGS) bottom sub cell to build a tandem cell. The multi-junction solar cell behavior is improved by engineering the technological and physical parameters of the perovskite and HTM. The results show that an n-p heterojunction PSC structure with an ETM free could be a good candidate for the traditional n-i-p structure. Because of such investigations, the performance of the proposed ETM-free PSC/CIGS cell could be designed to reach a PCE as high as 35.36%.

Keywords: CIGS; perovskites; efficient multi-junction solar cell; SCAPS-1D; zinc oxide (ZnO)



Citation: Salah, M.M.; Zekry, A.; Shaker, A.; Abouelatta, M.; Mousa, M.; Saeed, A. Investigation of Electron Transport Material-Free Perovskite/CIGS Tandem Solar Cell. *Energies* 2022, *15*, 6326. https:// doi.org/10.3390/en15176326

Academic Editor: Adalgisa Sinicropi

Received: 22 July 2022 Accepted: 13 August 2022 Published: 30 August 2022

**Publisher's Note:** MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



**Copyright:** © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/).

## 1. Introduction

Nowadays, the need for energy is increasing rapidly [1,2]. Clean energy, especially produced by solar cells, presents a promising solution [3]. The market for photovoltaics is now dominated by multi-crystalline and monocrystalline solar cells made of crystallized silicon. Solar cells made of crystalline silicon are currently more than 25% efficient [4,5]. Furthermore, thin film solar cells produced from CIGS are extremely competitive and have a PCE of 23.35% [6]. PSCs have also been developed, demonstrating cursory progress, and giving the field of photovoltaics new directions. PSC devices now have an efficiency record of more than 22% [7], and the advancement of PSCs in the last few years shows simulation results that exceed 30% [8]. Perovskite-based cells perform better due to low recombination losses, high extinction coefficients, a long diffusion length, a decent short circuit current, and energy gap adjustability.

ETM-free PSCs are very promising cells because they offer simple architectures, are low-cost, and have a high performance [9]. Because of the imbalanced charge transfer rate and the lack of a permanent built-in field in the absence of an ETL, ETL-free perovskite solar cells suffer from significant hysteresis and unsteady stabilized-power output [10]. The surface modification of an FTO substrate with a self-assembled fullerene monolayer (SAM), on the other hand, can improve device performance and reduce PSC hysteresis [11,12]. FTO effects on cells can be treated using different methods, one of which is produced for PSCs in a simplified configuration of glass/FTO–TMAH/perovskite/spiro-OMeTAD/Au using a modified FTO surface with tetramethylammonium hydroxide (TMAH). The increased device performance may be attributed to the improved charge extraction/transport, lower trap density, and lower charge recombination rate at the FTO/perovskite interface and in the perovskite layer, which displays up to 20.1% efficiency experimentally [13].

In 1961, in a single-junction solar cell with an energy gap of 1.34 eV, a maximum PCE of 33.7% was theoretically reported [14]. As the single junction can absorb photons with

the same energy gap or higher of the materials being utilized, the corresponding cells have a constrained performance. The remainder of the incident photons are not absorbed, and the spectrum with higher energy loses the excess energy because of the thermalization process. This limitation could be resolved by tandem solar cells as they are made up of sub cells that perform better than single-junction solar cells and absorb different wavelengths of the light spectrum [15]. The sub cell with a high energy gap is placed at the top as it absorbs the shorter wavelength radiation of the incident solar radiation, while the longer wavelength part of the incident spectrum, which is not absorbed by the top sub cell, will be transferred towards the bottom cell. The maximum theoretical PCE has been found to be more than 68% for infinity sub cells [16].

Tandem cells with two sub cells can be built through various methods; either fourterminal mechanically stacked and spectrum split, three-terminal, or two-terminal monolithic and mechanically stacked devices, as illustrated in Figure 1 [17]. The fundamental electrical constraint in these cells is the current in the two-terminal (2T) tandem cells. The cell performance is restricted by matching the current between the sub cells. In threeterminals (3T) tandem cells, the sub cells can be connected in parallel. The lowest voltage in this pair limits the voltage of this type of tandem cell. In four-terminal (4T) tandem cells, independent sub cells with their anodes and cathodes are connected electrically by an external circuit. The four-terminal spectrum split is still fundamental for the four-terminal device, and the light spectrum is separated using a dichroic filter. The additional expenses of the filter and the four terminals restrict the architecture's practical potential.



Figure 1. Tandem solar cell types: (a) two terminals monolithic, (b) two terminals mechanically stacked, (c) three terminals monolithic, (d) four terminals mechanically stacked (used in this work), and (e) four terminals spectrum-split.

The performance of solar cells can be simulated, assessed, and estimated through the use of simulation tools. Additionally, simulation technologies help designers save time and money by optimizing several architectural and material characteristics. It is well known that SCAPS-1D is a useful simulator for designing different kinds of solar cells [18]. Consequently, it has been used and validated against experimental works [8]. Up to seven layers of solar cells may be simulated using SCAPS-1D [19]. In addition, almost all material parameters, such as energy gaps, affinities, thicknesses, and others, may be tuned [20].

Most works on perovskite/CIGS tandem cells have concentrated on the mechanically stacked design. To enhance the use of the solar spectrum, a semitransparent PSC is placed on top of a CIGS device [21]. Because of the modest capital expenditure required for this technology, current technologies may be upgraded, providing an easy path to commercialization [22]. The four-terminal design is commonly used because it eliminates the requirement for the complicated current matching condition for two-terminal cells. The

utilization of two distinct substrates decreases the constraints on the manufacturing process and cell design [21]. A PCE of 15.5% has been reported using solution-processed PSC/CIGS tandem cells [23]. Because mixed-halide perovskites have a poor stability [24], a semitransparent MAPbI<sub>3</sub> cell with 12.7% PCE was layered atop a 17% CIGS cell to generate a PCE of 18.6% efficient tandem cell [22]. The replacement of the ZnO:Al TCO with sputtered In<sub>2</sub>O<sub>3</sub>:H resulted in a 20.5% tandem cell [25]. A tandem device with a PCE of 20.7% has been reported [26]. Improved tandem PCEs of up to 22.1% by employing a transparent contact consisting of MoO<sub>3</sub> and ZnO:Al was achieved [27]. Recently, Si/CIGS four-terminal tandem solar cells have exceeded a PCE of 25% [28]. According to a comprehensive optical investigation of perovskite/CIGS tandem cells, a PCE of 29% was reported in the literature [29].

In this paper, a PSC/CIGS four-terminal mechanically stacked tandem cell was formed by two independently designed cells, which allowed for a more efficient construction procedure. Each cell created its electrical output, necessitating the need for four-terminal connections. Iodide/chloride mixed halide perovskite MAPbI<sub>3-x</sub>Cl<sub>x</sub>, produced by incorporating Cl into MAPbI<sub>3</sub>, was used because its films exhibit a higher thermal stability and longer diffusion lengths [8], besides its tunable bandgap energy. In addition, a PSC without an ETM as a top cell replacing the conventional cell was proposed. It demonstrated a better performance. Furthermore, the influence of the thickness and doping of the sub cells' thin films was investigated in order to increase the PCE. The impact of the defect density and energy gap of the absorber films in the sub cells was studied.

The remainder of this paper is arranged as follows. At the beginning of Section 2, it is discussed how the tandem solar cell was initially conceived and how it has been explored. An n-i-p PSC calibration is shown in Section 2.1, as a CIGS solar cell with experimental cells. In Section 3.1.1, a PSC with ETM free is proposed. Moreover, an optimization of the proposed cell is presented. Section 3.1.2 shows the optimization of the calibrated CIGS cell. Section 3.1.3 compares the calibrated cells and the optimized cells. The optimized tandem device is illustrated in Section 3.2. Furthermore, Section 3.3 gives a comparative study between the suggested tandem cell and recent studies. Finally, Section 4 draws the conclusions.

#### 2. Materials and Methods

In the proposed tandem cell, PSC served as a top sub cell, and a GIGS solar cell served as a bottom sub cell, as illustrated in Figure 2a. The energy diagrams of the two sub cells are illustrated in Figure 2b (for the top cell) and Figure 2c (for the bottom cell). The top sub cell is composed of the perovskite layer stacked between the HTM and ETM. After calibration against an experimental cell, a PSC without ETM will be proposed.

The FTO is an optical transparent cathode, permitting light to cross the layers and transport the electrons produced to the cell's contacts. In the front of the CIGS absorber material, an n-type window layer consisting of two layers of zinc oxide (ZnO) and Cadmium sulfide (CdS) exists. Because of its characteristics, mainly tunable  $E_g$ , CIGS is an efficient absorber in the bottom sub cell. The transferred spectrum of the top cell towards the bottom cell, and the absorption coefficient ( $\alpha$ ) are given by Equations (1) and (2) [30,31]. The definitions of the parameters of Equations (1) and (2), and their units are listed in Table S1.

$$S(\lambda) = S_o(\lambda). \prod_{x=1}^n e^{-\alpha_x d_x} .$$
(1)

$$\alpha(E) = A_{\alpha} \sqrt{h\nu - E_g} \tag{2}$$



**Figure 2.** (a) The proposed perovskite/CIGS tandem device configuration and the energy levels of (b) the top cell and (c) the sub cell.

## 2.1. Validation of Physical Parameters Selection

A PSC with an ETM was modeled into SCAPS-1D. The results were validated with published experimental PSCs [32]. The design of the fabricated cell was a glass substrate, FTO (work function = 4 eV), titanium dioxide (TiO<sub>2</sub>) as an ETM, MAPbI<sub>3-x</sub>CI<sub>x</sub> as an absorber layer, Spiro-OMeTAD as an HTM, and finally an anode metal contact [32]. The material parameters utilized in the SCAPS-1D simulator are given in Table 1, while the ETM/absorber and absorber/HTM interfacial parameters are recorded in Table S2. To accomplish the practical considerations, a neutral defect with Gaussian distribution was invoked [33]. A 300 K temperature and air mass of 1.5 global (AM 1.5G) as the incident spectrum were utilized for all simulations. Thermal velocities of the carriers of 10<sup>7</sup> (cm/s) were used [34]. The absorption coefficients ( $\alpha$ ) were computed using Equation (2).

Parameters	FTO [36]	MAPbI <sub>3-x</sub> CI <sub>x</sub> [37,38]	Spiro-OMeTAD [10,39,40]	TiO <sub>2</sub> [38,41,42]	CIGS [35,43–45]	CdS [44]	ZnO [44]	ZnO-Al [44]
Band gap energy $E_g$ (eV)	3.5	1.55	3	3	1.04-1.67	2.45	3.30	3.30
Thickness (nm)	200	Fitting	200	50	2000-3000	50	100	400
Relative permittivity $\varepsilon_r$	9	6.5	3	10	13.6	10.0	9.0	9.0
Electron affinity $\chi$ (eV)	4	3.9	2.35	4	4.5	4.4	4.6	4.6
Effective conduction band density $N_c$ (cm <sup>-3</sup> )				$2.2 imes10^{18}$				$3 imes 10^{18}$
Electron mobility $\mu_e$ (cm <sup>-2</sup> V <sup>-1</sup> s <sup>-1</sup> )	20	2	$2 imes 10^{-4}$	20		100		

**Table 1.** The SCAPS-1D top and bottom sub cells' material parameters.

Parameters	FTO [36]	MAPbI <sub>3-x</sub> CI <sub>x</sub> [37,38]	Spiro-OMeTAD [10,39,40]	TiO <sub>2</sub> [38,41,42]	CIGS [35,43–45]	CdS [44]	ZnO [44]	ZnO-Al [44]
Donor concentration $N_D$ (cm <sup>-3</sup> )	$2\times 10^{19}$	0	0	$10^{18}$	0	10 <sup>20</sup>	1017	10 <sup>20</sup>
Effective valence band density $N_v$ (cm <sup>-3</sup> )	18	$8 \times 10^{17}$			$1.8 imes10^{19}$			$1.7 imes10^{19}$
Hole mobility $\mu_p \text{ (cm}^{-2} \text{ V}^{-1} \text{ s}^{-1} \text{)}$	10	2	$2 imes 10^{-4}$	10	25	25	25	31
Acceptor concentration $N_A$ (cm <sup>-3</sup> )	0	0	$2\times 10^{18}$	0	2×10 <sup>16</sup>	0	0	0
Defect density $N_t$ (cm <sup>-3</sup> )	10 <sup>15</sup>	$2 imes 10^{14}$	10 <sup>15</sup>	$10^{15}$	$10^{14}$	$10^{14}$ – $5 \times 10^{16}$	$10^{14}$	$10^{14} - 10^{16}$
Thermal velocity of electrons $v_{th,n}$ (cm/s)				107				$2.4  imes 10^7$
Thermal velocity of holes $v_{th,p}$ (cm/s)	-							$1.3  imes 10^7$

Table 1. Cont.

Figure 3a depicts the J-V characteristics of the experimental PSC with various thicknesses of the perovskite material versus the simulated one, while Figure 3b illustrates the J-V curves of the experimental PSC after optimization against the simulated PSC. The performance parameters (short circuit current density ( $J_{sc}$ ), open-circuit voltage ( $V_{oc}$ ), fill factor (FF), and PCE) of the simulation and the experimental work with different perovskite thicknesses, as well as the champion one, are recorded in Table S3, and Table 2, respectively. The simulation outputs were consistent with the experimentally reported ones.



**Figure 3.** The *J*–*V* characteristics of the proposed photovoltaic devices vs. the experimental cells: (a) PSC with different thicknesses [32], (b) the champion one of the PSCs [32], and (c) CIGS [35].

 Table 2. Comparison of the experimental PSC data [32], CIGS data [35], and simulations utilizing SCAPS-1D.

Absorber	Туре	PCE (%) $J_{sc}$ (mA/cm <sup>2</sup> )		$V_{oc}$ (V)	FF (%)
Perovskite	Experimental	19.41	23.80	1.09	75.16
	Simulation	19.41	23.50	1.09	75.55
CICC	Experimental	20.10	36.30	0.72	76.80
CIGS	Simulation	20.08	36.22	0.72	77.05

Furthermore, the CIGS cell was designed as a bottom sub cell of 4T multi-junction solar cells. So, firstly, the CIGS cell model was calibrated with the reported experimental results [35]. The parameters used for the calibration are given in Table 1, while the cell structure is displayed in Figure 2a. The J-V characteristics of both the experimental and

simulation CIGS devices are demonstrated in Figure 3c. The output metrics of the calibrated and the experimental cells are given in Table 2. The output parameters of the calibrated device were consistent with the experimentally reported characteristics and cell parameters. The good agreement validates the used physical parameters in the simulation for the two sub cells.

There was little difference between the simulated results and the experimental results in the PSC and CIGS cell. These differences could result from a minimal difference in the layers' thickness and some physical parameters, which were not given in the experimental work.

#### 3. Results and Discussions

#### 3.1. Optimization of the Sub Cells

In this section, the main material parameters of the top and bottom sub cells as single-junction cells are optimized.

#### 3.1.1. Optimization of the Top Sub cell

The doping of the materials in solar devices dramatically impacts the output performance. ETL has a stronger influence on the diffusion or carriers compared with the HTL [46]. Figure 4a illustrates the impact of ETM's  $N_D$  on the PCE. In PSCs, ETM doping has a low influence on the output performance when the absorber material has been doped [47]. Consequently, a PSC without ETM has been investigated in order to substitute the traditional PSC design to decrease the number of interfaces and layers. The perovskites could be doped *p*-type or *n*-type [48]. The doping density of perovskite could be adjusted between  $N_A$  of  $10^{14}$  cm<sup>-3</sup> and  $N_D$  of 7.6 ×  $10^{20}$  cm<sup>-3</sup> [48]. After removing the ETM layer, the output parameters were constant in the  $N_A$  range of  $0-10^{15}$  cm<sup>-3</sup>. Figure 4b illustrates the impact of the absorber film's  $N_D$  on the PCE with and without ETM. This work proposes a suitable doping level of  $1 \times 10^{13}$  cm<sup>-3</sup> for the perovskite active layer's  $N_D$ , achieving a PCE of 19.52%.

Because of the higher series resistance for the low doping concentration  $N_A$ , the performance metrics were low. Upon increasing the doping of HTM, the energy band offset between the perovskite layer and HTM also increased, which caused the diffusion current to rise significantly to the gradient of the doping concentration and caused particles to move according to Brownian motion—random thermal motion—from the regions with the highest to the lowest concentrations. Figure 4c depicted the effect of HTM's  $N_A$  on the PCE. The highest PCE was achieved beyond  $N_A$  of  $10^{19}$  cm<sup>-3</sup>. It was preferable to keep  $N_A$  at a low level to avoid high doping effects, such as band gap narrowing, the generation of deep Coulomb traps, and a reduction in mobility [49]. The output performance factors, PCE, FF,  $V_{oc}$ , and  $J_{sc}$ , when  $N_A$  of HTM was  $10^{19}$  cm<sup>-3</sup> were 20.05%, 77.38%, 1.1 V, and 23.51 mA/cm<sup>2</sup>, respectively. The effect of HTM thickness was also investigated.

Figure 4d depicts the impact of HTM's thickness on the PCE. The HTM's thickness has a minor effect on the performance parameters. It can be observed that as the thickness of HTM grew beyond 50 nm, the PCE slightly dropped. There was no change in PCE for thicknesses lower than 50 nm. Consequently, a layer thickness of 50 nm achieved a PCE of 20.08%, *Jsc* of 23.51 mA/cm<sup>2</sup>, and FF of 77.46%, and the same  $V_{oc}$  was selected.

Notably, performance characteristics were greatly influenced by the perovskite layer's defect concentration. The behavior of PSCs was significantly impacted by the quality of the photoactive material [50]. Photoelectrons were generated in the absorber thin film upon illumination. The lower quality of material implied a higher defect density, which resulted in increasing the non-radiative recombination losses [51]. This effect caused a higher SRH recombination rate, which was reflected in a deterioration in  $V_{oc}$  [52]. Figure 4e illustrates the fluctuation in PCE against the variation of  $N_t$ . Notably, reducing  $N_t$  decreased the recombination rates of carriers. As a result, a better performance was achieved at lower values of  $N_t$ . It was revealed that an  $N_t$  of  $10^9$  cm<sup>-3</sup> could be obtained [53]. However, as lowering  $N_t$  increased the cost,  $N_t$  of  $10^{12}$  cm<sup>-3</sup> could be selected as a compromise between



a high performance and low cost. When  $N_t$  was  $10^{12}$  cm<sup>-3</sup>, the key photovoltaic parameters were PCE = 24.64%, FF = 84.17%,  $V_{oc}$  = 1.24 V, and,  $J_{sc}$  = 23.61 mA/cm<sup>2</sup>.

**Figure 4.** Output PCE variation of the top sub cell depends on (**a**)  $N_D$  of the ETM, (**b**)  $N_D$  of the perovskite material with and without the ETM, (**c**)  $N_A$  of the HTM, (**d**) thickness of the HTM, and (**e**)  $N_t$  of the perovskite.

#### 3.1.2. Optimization of the Bottom Sub Cell

The doping concentration  $N_D$  of the CdS material was tested within the range of  $10^{15}-10^{18}$  cm<sup>-3</sup>. The PCE increased with the doping levels up to  $10^{17}$  cm<sup>-3</sup> and then slightly decreased. The PCE of the bottom sub cell with a CdS material doping concentration is shown in Figure 5a. The output parameters, PCE, FF,  $V_{oc}$ , and  $J_{sc}$ , when  $N_D$  of CdS was  $10^{17}$  cm<sup>-3</sup>, were 20.14%, 75.39%, 0.72 V, and 37.12 mA/cm<sup>2</sup>, respectively. Furthermore, the thickness of the CdS layer was tested up until 200 nm. The results showed that the PCE decreased with an increasing thickness, as illustrated in Figure 5b. Consequently, a film thickness of 10 nm was chosen with a PCE, FF, and  $J_{sc}$ , of 20.67%, 76.47%, and 37.52 mA/cm<sup>2</sup>, respectively, and without variation in  $V_{oc}$  of the previous step.

Moreover, the ZnO layer doping concentration was tested up to  $10^{20}$  cm<sup>-3</sup> as the CdS layer. Figure 5c shows the testing results of the bottom sub cell PCE with the ZnO layer doping level. PCE increased with the doping level up to about  $10^{19}$  cm<sup>-3</sup>. The doping of the ZnO layer should not be too high to impede the rapid recombination rate. On the other hand, the doping concentration should not be too low to impede decreasing the FF [54]. The performance metrics, PCE, FF, and  $J_{sc}$ , for  $N_D$  of ZnO of  $10^{19}$  cm<sup>-3</sup>, were 20.78%, 76.8%, 0.72 V, and 37.55 mA/cm<sup>2</sup>, respectively, and without variation in  $V_{oc}$  of the previous step. Furthermore, the PCE of the bottom sub cell was analyzed with ZnO film thickness of up to 300 nm, as displayed in Figure 5d. The PCE did not change up to 100 nm, and then decreased by a very small amount up to 200 nm, and was then fixed. So, the ZnO layer thickness variation had almost no effect on the bottom sub cell performance.



**Figure 5.** (a) Photovoltaic output parameters of the bottom sub cell depend on (a)  $N_D$  of the CdS layer, (b) thickness of the CdS material, (c)  $N_D$  of the ZnO layer, and (d) thickness of the ZnO layer.

Next, the CIGS absorber layer of the bottom sub cell doping level was checked in the range of  $10^{15}$ – $10^{20}$  cm<sup>-3</sup>. The PCE of the bottom sub cell with this variation of the doping concentration is illustrated in Figure 6a. The PCE increased with increasing the doping level. The highest PCE was achieved in the highest  $N_A$ , as shown in Figure 6a. However, as stated before, it was preferable to keep  $N_A$  at a low level because a high  $N_A$ creates deep Coulomb traps and, in turn, decreases mobility [49]. The performance key factors, PCE, FF,  $V_{oc}$ , and  $J_{sc}$ , for  $N_A$  of CIGS of  $10^{17}$  cm<sup>-3</sup> were 22.13%, 77.82%, 0.76 V, and 37.31 mA/cm<sup>2</sup>, respectively. In addition, the CIGS layer thickness of the bottom sub cell was tested up until 5  $\mu$ m. The PCE increased up to about 2.5  $\mu$ m and then was almost saturated, as displayed in Figure 6b. Consequently, a thickness of 2.5 µm was selected, with the same performance parameters as the previous step. The last test of the optimization of the bottom sub cell was testing of the cell PCE with a defect level. Figure 6c shows the PCE vs. the variation of the defect density in the range of  $10^{12}$ – $10^{15}$  cm<sup>-3</sup>. The PCE decreased by increasing the defect level by a small rate of up to  $10^{14}$  cm<sup>-3</sup> and then dropping by a high rate. Decreasing the defect concentration had a strong dependence on the quality of the fabrication process, which results in increased costs. Consequently,  $N_t$  of  $10^{14}$  cm<sup>-3</sup> was chosen to be a practical value with the same performance metrics as the previous step.



**Figure 6.** (a)  $N_A$  of the CIGS layer, (b) thickness of the CIGS layer, and (c)  $N_t$  of CIGS.

3.1.3. The Initial Sub Cells vs. the Optimized Sub Cells

Lowering the recombination rates at the ETM/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3-x</sub>CI<sub>x</sub>/HTM interfaces is a significant method to efficiently extract the carriers. The optimum valence band offset (VBO) and conduction band offset (CBO) to be 0–0.2 eV lower than and 0–0.3 eV higher than the VBO and CBO of the CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3-x</sub>CI<sub>x</sub>, for HTM and ETM, respectively [55,56]. VBO and CBO are given by (3) and (4), respectively [38,55,56].

$$VBO = (\chi_{HTL} + E_{g.HTL} - \chi_{pero.} - E_{g.pero.})$$
(3)

$$CBO = (\chi_{pero.} - \chi_{ETM})$$
(4)

where  $\chi_{HTL}$  is the affinity of the HTM and  $\chi_{pero.}$  is the absorber layer affinity. Considering the equation and perovskite affinity of 3.9 eV, and the  $E_g$  is 1.55 eV, the optimum VBO of the HTM lies between the values of 5.15 eV and 5.45 eV. This condition is satisfied with Spiro-OMeTAD as HTM. The optimum CBO of the ETM lies in the range of 3.9–4.2 eV because of the previous equation and the perovskite affinity. This condition is satisfied with the TiO<sub>2</sub> affinity, which is 4 eV. In addition, CBO is in the optimum range when removing the ETM as the affinity of FTO is 4 eV.

To give supplemental physical reasoning for the enhancement of the output parameters, Figure 7a,b illustrates the energy band profiles of the initial PSC and those of the optimum PSC with ETM free, respectively. As it can be inferred from these figures, the electrostatic potential between  $CH_3NH_3PbI_{3-x}CI_x$  and FTO films is better than the electric potential between  $CH_3NH_3PbI_{3-x}CI_x$  and TiO<sub>2</sub>. This improvement can speed up the separation of photon-generated carriers, lowering the recombination rate and improving the PSC metrics.



**Figure 7.** Energy band diagrams of the PSC: (**a**) before the optimization of doping, thickness, defect density; (**b**) after the optimization; and (**c**) the recombination rates of the initial and the optimized cells.

The variation of the performance factors could be clarified by observing the recombination rates of the initial and optimized cells. Figure 7c demonstrates the recombination rate (in cm<sup>-3</sup>·s<sup>-1</sup>) variations along the PSC distance. It is obvious from the figure that the recombination rate is high at the interface between perovskite/ETM, which can be prevented in the optimized cell. Furthermore, the recombination rate at the interface between HTM/perovskite after optimization is also lower than before optimization. In addition, the recombination rate in the absorber layer is reduced. The output performance trend supports the idea of removing the ETM from the PSC and showing our optimization's importance. Table 3 lists a comparison of PCEs for single-junction PSCs of calibrated PSC, optimized PSC without ETM, and other investigations.

Table 3. Comparison of PCEs of the latest PSCs.

ETM/HTM	PCE (%)
TiO <sub>2</sub> /CuI [57]	21.32
TiO <sub>2</sub> /CuI [58]	21.76
ZnOS/CuI [58]	26.11
PEDOT:PSS/HATNT [59]	18.10
PEDOT:PSS/TDTP [60]	18.20
TiO <sub>2</sub> /- [61]	25.15
nanoparticle based SnO <sub>2</sub> /Spiro-OMeTAD [28]	17.90
TiO <sub>2</sub> /Spiro-OMeTAD [32]	19.41
-/Spiro-OMeTAD [optimized]	27.13

For a more supplemental physical reasoning for the enhancement of the output parameters, Figure 8a,b illustrates the energy band diagrams of the initial CIGS cell and the optimized one. It can be inferred from these figures that the spike-like CBO effect, which resulted in lowering the FF, was solved after optimization. This improvement could speed up the separation of photogenerated carriers, reducing the recombination rate and enhancing the performance parameters. The improvement of the performance parameters could be justified by the observation of the recombination rates before and after optimization. In this regard, Figure 8c demonstrates the recombination rate was very high at the ZnO/CdS interface, which was decreased after optimization.



**Figure 8.** Energy band diagrams of the CIGS solar cell: (a) before the optimization of doping, thickness, defect density; (b) after the optimization; and (c) the recombination rates of the initial and the optimized cells.

#### 3.2. The Final Tandem Cell

Based on the preceding outcomes, the top sub cell used a glass substrate, TCO, an absorber layer of N-type  $CH_3NH_3PbI_{3-x}CI_x$ , and an HTM of Spiro-OMeTAD. The bottom sub cell that was used had CIGS as an absorber layer. The CIGS employed in the bottom sub

cell exhibited a high current density, which influenced the tandem cell's overall behavior in terms of current density and PCE. The energy gap of the perovskite material could be tuned from 1.5 to 1.63 eV [62,63], while the energy gap of CIGS could be tuned from 1.04 to 1.67 eV [43–45]. Decreasing the energy gap increased the amount of the absorbed spectrum. Figure 9a illustrates the PCE of the N-CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3-x</sub>CI<sub>x</sub> (without ETM)/CIGS tandem solar cell with various energy gaps of the absorbers of the sub cells. The top sub cell had a PCE of 27.74% when the absorber's  $E_g$  was 1.5 eV, and its thickness was 0.9 µm. The bottom sub cell had a PCE of 20.04% when the absorber's  $E_g$  was 1.04 eV with the transmitted spectrum of the top sub cell. The PCE of the tandem solar cell with these energy gaps was 34%. It can be concluded from Figure 9b that the highest PCE was at a 1.1 um thickness of the active thin film of the top sub cell. However, a thickness of 0.9 um was chosen with a PCE of 35.36% so as to be of more practical value with a low-cost fabrication [64,65]. Figure 9c shows the final tandem solar cell's structure in detail, including each layer's thickness and doping concentration.



**Figure 9.** Dependence of PCE of the tandem cell on (**a**) the energy gaps of the absorbers, (**b**) the thickness of the top sub cell absorber, (**c**) the final perovskite/*CIGS* tandem cell, (**d**) the output performance curves of the sub cells, tandem cell, J–V curves, and (**e**) QE curves.

The current density as a function of the voltage of the sub cells as an incident spectrum was AM 1.5G and of the bottom sub cell, as illuminated by the transmitted spectrum from the top sub cell, are illustrated in Figure 9d. Figure 9e shows the *QE* characteristics of the sub cells and the tandem cell. Figure 10a shows the materials used in the tandem cell absorption coefficients. At the same time, Figure 10b shows the absorbed spectrum of both sub cells with the incident AM 1.5G spectrum. According to the results, CIGS can absorb most of the transmitted spectrum up to 1200 nm when used as a bottom sub cell. This is larger than most of the other substances that can serve as bottom sub cell absorbers. This explains why the behavior of the tandem cell has improved.



**Figure 10.** (a) Absorption coefficients of the materials used in the final tandem cell, and (b) AM 1.5G spectrum with the absorbed spectrum of the sub cells.

#### 3.3. Comparison with the State of Art Published Results

The PCE of some recent tandem solar cells during the past several years is described in this section. In this context, Table 4 compares the results of this study and other published results. Even among tandem cells with more than two connections and double junction tandem cells, the suggested tandem cell has one of the greatest efficiencies.

PCE (%)	The Material of Top/Bottom Sub Cells	RefYear
25	Perovskite/CIGS	[28]-2020
25.7	Perovskite/C-Si	[28]-2020
29.8	Perovskite/Si	[66]-2022
30.2	Se/CZTSSe	[67]-2019
30.5	MAPbI <sub>3</sub> /CIGS	[68]-2020
31.1	GaInP/Si	<b>[69]-2020</b>
33.3	Triple-junction (Ga <sub>0.51</sub> In <sub>0.49</sub> P/GaAs/Si)	[67]-2018
35.36	MAPbI <sub>3-x</sub> Cl <sub>x</sub> without ETM/CIGS	This work
35.9	Triple-junction (GaInP/GaAs/Si)	[70]-2017
39.2	Six-junction (monolithic)	[34]-2017
30.2	Se/CZTSSe	[67]-2019

Table 4. A comparison of the suggested tandem cell with the state-of-the-art of published data.

## 4. Conclusions

The tandem multi-junction solar cells' performance exceeds single-junction cells because of their capability to absorb a broader spectrum. Here, we reported using a tandem solar cell that is based on perovskite and CIGS as top and bottom sub cells, respectively. The simulation of perovskite solar cells is firstly presented with TiO<sub>2</sub> as an ETM and Spiro-OMeTAD as an HTM. Then, a PSC without an ETM is proposed in order to achieve more stability and reduce the cost of the top sub cell. This structure has a simple design and shows superior output metrics. The main material parameters of the suggested Spiro-OMeTAD/MAPbI<sub>3-x</sub>Cl<sub>x</sub> perovskite solar cell without an HTM are studied in order to enhance the photovoltaic device's behavior. The doping, thickness of all layers, perovskite layer's defect concentration, and energy gap are investigated. The output performance parameters after optimization, for PCE, FF,  $V_{oc}$ , and  $J_{sc}$ , are 27.74% 80.71%, 1.23 V, and 28 mA/cm<sup>2</sup>, respectively. Moreover, a CIGS sub cell is calibrated with a practical cell. In addition, the doping and the thickness of all layers, besides the CIGS layer's defect concentration are studied. After optimization, the CIGS cell has performance metrics when illuminated by the transmitted spectrum of the top sub cell, for PCE, FF,  $V_{oc}$ , and  $J_{sc}$ , which are 20.04%, 76.34%, 0.57 V, and 18.31 mA/cm<sup>2</sup>, respectively. This CIGS cell is utilized as a bottom sub cell of the tandem cell. All of the applied improvements on the sub cells, besides the energy gaps of the absorbers, reflect on the PCE of the suggested tandem cell to be 35.36%. This design shows a higher performance than many more complex tandem cells. The tandem cell that has been proposed here exhibits one of the tandem cells' finest performances, despite being simpler.

**Supplementary Materials:** The following supporting information can be downloaded at: https: //www.mdpi.com/article/10.3390/en15176326/s1. Table S1: Physical parameters of the incident, transmitted spectrum definitions, and their units; Table S2: Parameters of defect interfaces; Table S3: Comparison of experimental PSC data [32], and simulations utilizing SCAPS-1D with different perovskite thicknesses. Reference [71] is cited in the Supplementary Materials.

Author Contributions: Conceptualization, M.M.S., M.A., A.S. (Ahmed Shaker), M.M., and A.S. (Ahmed Saeed); methodology, M.M.S., M.A., A.S. (Ahmed Shaker), M.M., and A.S. (Ahmed Saeed); validation and formal analysis, M.M.S., M.A., A.S. (Ahmed Shaker), M.M., and A.S. (Ahmed Saeed); visualization, M.M.S. and M.M.; investigation, all authors; writing—original draft preparation, M.M.S., M.A., A.S. (Ahmed Shaker), M.M., and A.S. (Ahmed Shaker), M.M., and editing, all authors; supervision, A.Z., M.A., A.S. (Ahmed Shaker), and A.S. (Ahmed Saeed); All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

**Data Availability Statement:** No new data were created or analyzed in this study. Data sharing does not apply to this article.

Conflicts of Interest: The authors declare no conflict of interest.

#### References

- Sahbel, A.; Hassan, N.; Abdelhameed, M.M.; Zekry, A. Experimental Performance Characterization of Photovoltaic Modules Using DAQ. *Energy Procedia* 2013, 36, 323–332. [CrossRef]
- Zekry, A. A road map for transformation from conventional to photovoltaic energy generation and its challenges. J. King Saud Univ. Eng. Sci. 2020, 32, 407–410. [CrossRef]
- Gielen, D.; Boshell, F.; Saygin, D.; Bazilian, M.D.; Wagner, N.; Gorini, R. The role of renewable energy in the global energy transformation. *Energy Strateg. Rev.* 2019, 24, 38–50. [CrossRef]
- Okil, M.; Salem, M.S.; Abdolkader, T.M.; Shaker, A. From Crystalline to Low-cost Silicon-based Solar Cells: A Review. *Silicon* 2021, 14, 1895–1911. [CrossRef]
- Yoshikawa, K.; Kawasaki, H.; Yoshida, W.; Irie, T.; Konishi, K.; Nakano, K.; Uto, T.; Adachi, D.; Kanematsu, M.; Uzu, H.; et al. Silicon heterojunction solar cell with interdigitated back contacts for a photoconversion efficiency over 26%. *Nat. Energy* 2017, 2, 17032. [CrossRef]
- Nakamura, M.; Yamaguchi, K.; Kimoto, Y.; Yasaki, Y.; Kato, T.; Sugimoto, H. Cd-Free Cu(In,Ga)(Se,S)2 thin-film solar cell with record efficiency of 23.35%. *IEEE J. Photovolt.* 2019, *9*, 1863–1867. [CrossRef]
- Yang, W.S.; Park, B.W.; Jung, E.H.; Jeon, N.J.; Kim, Y.C.; Lee, D.U.; Shin, S.S.; Seo, J.; Kim, E.K.; Noh, J.H.; et al. Iodide management in formamidinium-lead-halide-based perovskite layers for efficient solar cells. *Science* 2017, 356, 1376–1379. [CrossRef]
- Salah, M.M.; Abouelatta, M.; Shaker, A.; Hassan, K.M.; Saeed, A. A comprehensive simulation study of hybrid halide perovskite solar cell with copper oxide as HTM. *Semicond. Sci. Technol.* 2019, 34, 115009. [CrossRef]
- Han, Q.; Ding, J.; Bai, Y.; Li, T.; Ma, J.Y.; Chen, Y.X.; Zhou, Y.; Liu, J.; Ge, Q.Q.; Chen, J.; et al. Carrier Dynamics Engineering for High-Performance Electron-Transport-Layer-free Perovskite Photovoltaics. *Chem* 2018, 4, 2405–2417. [CrossRef]
- Yu, H.; Lee, J.W.; Yun, J.; Lee, K.; Ryu, J.; Lee, J.; Hwang, D.; Kim, S.K.; Jang, J. Outstanding Performance of Hole-Blocking Layer-Free Perovskite Solar Cell Using Hierarchically Porous Fluorine-Doped Tin Oxide Substrate. *Adv. Energy Mater.* 2017, 7, 1700749. [CrossRef]

- Valles-Pelarda, M.; Hames, B.C.; Inés García-Benito, I.; Almora, O.; Molina-Ontoria, A.; Sánchezsánchez, R.S.; Garcia-Belmonte, G.; Martín, N.; Mora-Sero, I. Analysis of the hysteresis behavior of perovskite solar cells with interfacial fullerene self-assembled monolayers. J. Phys. Chem. Lett. 2016, 7, 4622–4628. [CrossRef]
- Lamberti, F.; Gatti, T.; Menna, E.; Petrozza, A.; Topolovsek, P.; Lamberti, F.; Gatti, T.; Cito, A.; Ball, J.M.; Menna, E.; et al. Functionalization of transparent conductive oxide electrode for TiO 2-free perovskite solar cells. *J. Mater. Chem. A* 2017, *5*, 11882–11893. [CrossRef]
- Huang, C.; Lin, P.; Fu, N.; Liu, C.; Xu, B.; Sun, K.; Wang, D.; Zeng, X.; Ke, S. Facile fabrication of highly efficient ETL-free perovskite solar cells with 20% efficiency by defect passivation and interface engineering. *Chem. Commun.* 2019, 55, 2777–2780. [CrossRef] [PubMed]
- 14. Shockley, W.; Queisser, H.J. Detailed balance limit of efficiency of p-n junction solar cells. J. Appl. Phys. 1961, 32, 510–519. [CrossRef]
- Yasodharan, R.; Senthilkumar, A.P.; Mohankumar, P.; Ajayan, J.; Sivabalakrishnan, R. Investigation and influence of layer composition of tandem perovskite solar cells for applications in future renewable and sustainable energy. *Optik* 2020, 212, 164723. [CrossRef]
- 16. De Vos, A. Detailed balance limit of the efficiency of tandem solar cells. J. Phys. D Appl. Phys. 1980, 13, 839–846. [CrossRef]
- 17. Todorov, T.; Gunawan, O.; Guha, S. A road towards 25% efficiency and beyond: Perovskite tandem solar cells. *Mol. Syst. Des. Eng.* **2016**, *1*, 370–376. [CrossRef]
- Abdelaziz, W.; Zekry, A.; Shaker, A.; Abouelatta, M. Numerical study of organic graded bulk heterojunction solar cell using SCAPS simulation. Sol. Energy 2020, 211, 375–382. [CrossRef]
- 19. Burgelman, M.; Decock, K.; Khelifi, S.; Abass, A. Advanced electrical simulation of thin film solar cells. *Thin Solid Films* **2013**, 535, 296–301. [CrossRef]
- 20. Burgelman, M.; Decock, K.; Niemegeers, A.; Verschraegen, J.; Degrave, S. SCAPS Manual; University of Gent: Ghent, Belgium, 2014.
- Yun, S.; Qin, Y.; Uhl, A.R.; Vlachopoulos, N.; Yin, M.; Li, D.; Han, X.; Hagfeldt, A. New-generation integrated devices based on dye-sensitized and perovskite solar cells. *Energy Environ. Sci.* 2018, 11, 476–526. [CrossRef]
- Bailie, C.D.; Greyson Christoforo, M.; Mailoa, J.P.; Bowring, A.R.; Unger, E.L.; Nguyen, W.H.; Burschka, J.; Pellet, N.; Lee, J.Z.; Grätzel, M.; et al. Semi-transparent perovskite solar cells for tandems with silicon and CIGS. *Energy Environ. Sci.* 2018, *8*, 956–963. [CrossRef]
- Yang Michael, Y.; Chen, Q.; Hsieh, Y.T.; Bin Song, T.; De Marco, N.; Zhou, H.; Yang, Y. Multilayer Transparent Top Electrode for Solution Processed Perovskite/Cu(In,Ga)(Se,S)2 Four Terminal Tandem Solar Cells. ACS Nano 2015, 9, 7714–7721. [CrossRef]
- 24. Hoke, E.T.; Slotcavage, D.J.; Dohner, E.R.; Bowring, A.R.; Karunadasa, H.I.; Mcgehee, M.D. Reversible photo-induced trap formation in mixed-halide hybrid perovskites for photovoltaics. *Chem. Sci.* **2015**, *6*, 613–617. [CrossRef]
- Fu, F.; Feurer, T.; Jäger, T.; Avancini, E.; Bissig, B.; Yoon, S.; Buecheler, S.; Tiwari, A.N. ARTICLE Low-temperature-processed efficient semi-transparent planar perovskite solar cells for bifacial and tandem applications. *Nat. Commun.* 2015, *6*, 8932. [CrossRef]
- 26. Guchhait, A.; Dewi, H.A.; Leow, S.W.; Wang, H.; Han, G.; Bin Suhaimi, F.; Mhaisalkar, S.; Wong, L.H.; Mathews, N. Over 20% Efficient CIGS-Perovskite Tandem Solar Cells. *ACS Energy Lett.* **2017**, *2*, 807–812. [CrossRef]
- 27. Kranz, L.; Abate, A.; Feurer, T.; Fu, F.; Avancini, E.; Löckinger, J.; Reinhard, P.; Zakeeruddin, S.M.; Grätzel, M.; Buecheler, S.; et al. High-efficiency polycrystalline thin film tandem solar cells. *J. Phys. Chem. Lett.* **2015**, *6*, 2676–2681. [CrossRef]
- Gharibzadeh, S.; Hossain, I.M.; Fassl, P.; Nejand, B.A.; Abzieher, T.; Schultes, M.; Ahlswede, E.; Jackson, P.; Powalla, M.; Schäfer, S.; et al. 2D/3D Heterostructure for Semitransparent Perovskite Solar Cells with Engineered Bandgap Enables Efficiencies Exceeding 25% in Four-Terminal Tandems with Silicon and CIGS. *Adv. Funct. Mater.* 2020, 30, 1909919. [CrossRef]
- 29. Chen, C.-W.; Hsiao, S.-Y.; Chen, C.-Y.; Kang, H.-W.; Huang, Z.-Y.; Lin, H.-W. Optical properties of organometal halide perovskite thin fi lms and general device structure design rules for perovskite single and tandem solar cells. *J. Mater. Chem. A* 2015, *3*, 9152–9159. [CrossRef]
- Kim, K.; Gwak, J.; Ahn, S.K.; Eo, Y.J.; Park, J.H.; Cho, J.S.; Kang, M.G.; Song, H.E.; Yun, J.H. Simulations of chalcopyrite/c-Si tandem cells using SCAPS-1D. Sol. Energy 2017, 145, 52–58. [CrossRef]
- 31. Mandadapu, U.; Vedanayakam, S.V.; Thyagarajan, K. Simulation and Analysis of Lead based Perovskite Solar Cell using SCAPS-1D. *Indian J. Sci. Technol.* **2017**, *10*, 65–72. [CrossRef]
- 32. Ding, Y.; Shi, B.; Yao, X.; Fan, L.; Luo, J.; Wei, C.; Zhang, D.; Wang, G.; Sheng, Y.; Chen, Y.; et al. Elucidating the role of chlorine in perovskite solar cells. *J. Mater. Chem. A* 2017, *5*, 7423–7432. [CrossRef]
- Samiee, M.; Konduri, S.; Ganapathy, B.; Kottokkaran, R.; Abbas, H.A.; Kitahara, A.; Joshi, P.; Zhang, L.; Noack, M.; Dalal, V. Defect density and dielectric constant in perovskite solar cells. *Appl. Phys. Lett.* 2014, 105, 153502. [CrossRef]
- Li, X.; Yang, J.; Jiang, Q.; Chu, W.; Zhang, D.; Zhou, Z.; Xin, J. Synergistic Effect to High-Performance Perovskite Solar Cells with Reduced Hysteresis and Improved Stability by the Introduction of Na-Treated TiO2 and Spraying-Deposited CuI as Transport Layers. ACS Appl. Mater. Interfaces 2017, 9, 41354–41362. [CrossRef]
- Jackson, P.; Hariskos, D.; Lotter, E.; Paetel, S.; Wuerz, R.; Menner, R.; Wischmann, W.; Powalla, M. New world record efficiency for Cu(In,Ga)Se2 thin-film solar cells beyond 20%. *Prog. Photovolt. Res. Appl.* 2011, 19, 894–897. [CrossRef]

- Basyoni, M.S.S.; Salah, M.M.; Mousa, M.; Shaker, A.; Zekry, A.; Abouelatta, M.; Alshammari, M.T.; Al-Dhlan, K.A.; Gontrand, C. On the Investigation of Interface Defects of Solar Cells: Lead-Based vs Lead-Free Perovskite. *IEEE Access* 2021, 9, 130221–130232. [CrossRef]
- Etgar, L.; Gao, P.; Xue, Z.; Peng, Q.; Chandiran, A.K.; Liu, B.; Nazeeruddin, M.K.; Grätzel, M. Mesoscopic CH 3NH 3PbI 3/TiO 2 heterojunction solar cells. J. Am. Chem. Soc. 2012, 134, 17396–17399. [CrossRef] [PubMed]
- Bansal, S.; Aryal, P. Evaluation of new materials for electron and hole transport layers in perovskite-based solar cells through SCAPS-1D simulations. In Proceedings of the 2016 IEEE 43rd Photovoltaic Specialists Conference (PVSC), Portland, OR, USA, 5–10 June 2016; pp. 0747–0750. [CrossRef]
- 39. Gupta, G.K.; Dixit, A. Theoretical studies of single and tandem Cu2ZnSn(S/Se)4 junction solar cells for enhanced efficiency. *Opt. Mater.* **2018**, *82*, 11–20. [CrossRef]
- 40. Madan, J.; Shivani; Pandey, R.; Sharma, R. Device simulation of 17.3% efficient lead-free all-perovskite tandem solar cell. *Sol. Energy* **2020**, *197*, 212–221. [CrossRef]
- 41. Du, H.-J.; Wang, W.-C.; Zhu, J.-Z. Device simulation of lead-free CH3NH3SnI3 perovskite solar cells with high efficiency. *Chin. Phys. B* **2016**, *25*, 108802. [CrossRef]
- Niemegeers, A.; Burgelman, M. Numerical modelling of ac-characteristics of CdTe and CIS solar cells. In Proceedings of the Conference Record of the Twenty Fifth IEEE Photovoltaic Specialists Conference, Washington, DC, USA, 13–17 May 1996. [CrossRef]
- 43. Asaduzzaman, M.; Hasan, M.; Bahar, A.N. An investigation into the effects of band gap and doping concentration on Cu(In,Ga)Se2 solar cell efficiency. *Springerplus* **2016**, *5*, 578. [CrossRef]
- 44. Pudov, A.O.; Kanevce, A.; Al-Thani, H.A.; Sites, J.R.; Hasoon, F.S. Secondary barriers in CdS- CuIn1-x Gax Se2 solar cells. *J. Appl. Phys.* 2005, 97, 064901. [CrossRef]
- 45. Tverjanovich, A.; Borisov, E.N.; Vasilieva, E.S.; Tolochko, O.V.; Vahhi, I.E.; Bereznev, S.; Tveryanovich, Y.S. CuInSe2 thin films deposited by UV laser ablation. *Sol. Energy Mater. Sol. Cells* **2006**, *90*, 3624–3632. [CrossRef]
- Mahon, N.S.; Korolik, O.V.; Khenkin, M.V.; Arnaoutakis, G.E.; Galagan, Y.; Soriūtė, V.; Litvinas, D.; Ščajev, P.; Katz, E.A.; Mazanik, A.V. Photoluminescence kinetics for monitoring photoinduced processes in perovskite solar cells. *Sol. Energy* 2020, 195, 114–120. [CrossRef]
- 47. Salah, M.M.; Zekry, A.; Abouelatta, M.; Shaker, A.; Mousa, M.; Amer, F.Z.; Mubarak, R.I.; Saeed, A. High-Efficiency Electron Transport Layer-Free Perovskite/GeTe Tandem Solar Cell: Numerical Simulation. *Crystals* **2022**, *12*, 878. [CrossRef]
- 48. Wang, Q.; Shao, Y.; Xie, H.; Lyu, L.; Liu, X.; Gao, Y.; Huang, J. Qualifying composition dependent p and n self-doping in CH3NH3PbI3. *Appl. Phys. Lett.* **2014**, *105*, 163508. [CrossRef]
- 49. Tan, K.; Lin, P.; Wang, G.; Liu, Y.; Xu, Z.; Lin, Y. Controllable design of solid-state perovskite solar cells by SCAPS device simulation. *Solid-State Electron.* **2016**, *126*, 75–80. [CrossRef]
- 50. Kim, H.; Lim, K.G.; Lee, T.W. Planar heterojunction organometal halide perovskite solar cells: Roles of interfacial layers. *Energy Environ. Sci.* **2016**, *9*, 12–30. [CrossRef]
- Zekry, A.; Shaker, A.; Salem, M. Solar Cells and Arrays: Principles, Analysis, and Design. *Adv. Renew. Energies Power Technol.* 2018, 1, 3–56. [CrossRef]
- 52. Kirchartz, T.; Krückemeier, L.; Unger, E.L. Research Update: Recombination and open-circuit voltage in lead-halide perovskites. *APL Mater.* **2018**, *6*, 100702. [CrossRef]
- Shi, D.; Adinolfi, V.; Comin, R.; Yuan, M.; Alarousu, E.; Buin, A.; Chen, Y.; Hoogland, S.; Rothenberger, A.; Katsiev, K.; et al. Low trap-state density and long carrier diffusion in organolead trihalide perovskite single crystals. *Science* 2015, 347, 519–522. [CrossRef]
- 54. Salem, M.S.; Zekry, A.; Shaker, A.; Abouelatta, M.; Abdolkader, T.M. Performance enhancement of a proposed solar cell microstructure based on heavily doped silicon wafers. *Semicond. Sci. Technol.* **2019**, *34*, 035012. [CrossRef]
- 55. Salem, M.S.; Shaker, A.; Zekry, A.; Abouelatta, M.; Alanazi, A.; Alshammari, M.T.; Gontand, C. Analysis of Hybrid Hetero-Homo Junction Lead-Free Perovskite Solar Cells by SCAPS Simulator. *Energies* **2021**, *14*, 5741. [CrossRef]
- Minemoto, T.; Murata, M. Theoretical analysis on effect of band offsets in perovskite solar cells. Sol. Energy Mater. Sol. Cells 2015, 133, 8–14. [CrossRef]
- 57. Haider, S.Z.; Anwar, H.; Wang, M. A comprehensive device modelling of perovskite solar cell with inorganic copper iodide as hole transport material. *Semicond. Sci. Technol.* **2018**, *33*, 035001. [CrossRef]
- 58. Salah, M.M.; Hassan, K.M.; Abouelatta, M.; Shaker, A. A comparative study of different ETMs in perovskite solar cell with inorganic copper iodide as HTM. *Optik* **2019**, *178*, 958–963. [CrossRef]
- Wang, N.; Zhao, K.; Ding, T.; Liu, W.; Ahmed, A.S.; Wang, Z.; Tian, M.; Sun, X.W.; Zhang, Q. Improving Interfacial Charge Recombination in Planar Heterojunction Perovskite Photovoltaics with Small Molecule as Electron Transport Layer. *Adv. Energy Mater.* 2017, *7*, 1700522. [CrossRef]
- Gu, P.-Y.; Wang, N.; Wang, C.; Zhou, Y.; Long, G.; Tian, M.; Chen, W.; Sun, X.W.; Kanatzidis, M.G.; Zhang, Q. Pushing up the efficiency of planar perovskite solar cells to 18.2% with organic small molecules as the electron transport layer. *J. Mater. Chem. A* 2017, *5*, 7339–7344. [CrossRef]

- Lin, L.; Li, P.; Jiang, L.; Kang, Z.; Yan, Q.; Xiong, H.; Lien, S.; Zhang, P.; Qiu, Y.; Energy, S.L.-S.; et al. Boosting efficiency up to 25% for HTL-free carbon-based perovskite solar cells by gradient doping using SCAPS simulation. *Sol. Energy* 2021, 215, 328–334. [CrossRef]
- Chae, J.; Dong, Q.; Huang, J.; Centrone, A. Chloride Incorporation Process in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>-xClx Perovskites via Nanoscale Bandgap Maps. *Nano Lett.* 2015, 15, 8114–8121. [CrossRef]
- 63. Iefanova, A.; Adhikari, N.; Dubey, A.; Khatiwada, D.; Qiao, Q. Lead free CH3NH3SnI3 perovskite thin-film with p-type semiconducting nature and metal-like conductivity. *AIP Adv.* **2016**, *6*, 085312. [CrossRef]
- 64. Jäger, K.; Tillmann, P.; Katz, E.A.; Becker, C. Perovskite/Silicon Tandem Solar Cells: Effect of Luminescent Coupling and Bifaciality. *Sol. RRL* 2021, *5*, 2000628. [CrossRef]
- Köhnen, E.; Wagner, P.; Lang, F.; Cruz, A.; Li, B.; Roß, M.; Jošt, M.; Morales-Vilches, A.B.; Topič, M.; Stolterfoht, M.; et al. 27.9% Efficient Monolithic Perovskite/Silicon Tandem Solar Cells on Industry Compatible Bottom Cells. Sol. RRL 2021, 5, 2100244. [CrossRef]
- 66. Tockhorn, P.; Berlin, H.-Z.; Sutter, J.; Cruz, A.; Wagner, P.; Jäger, K.; Yoo, D.; Lang, F.; Grischek, M.; Li, B.; et al. Nano-optical designs enhance monolithic perovskite/silicon tandem solar cells toward 29.8% efficiency. *Res. Sq.* **2022**, *49*, 1–16. [CrossRef]
- 67. Ferhati, H.; Djeffal, F. Exceeding 30% efficiency for an environment-friendly tandem solar cell based on earth-abundant Se/CZTS materials. *Phys. E Low-Dimens. Syst. Nanostruct.* **2019**, *109*, 52–58. [CrossRef]
- Mousa, M.; Salah, M.M.; Amer, F.Z.; Saeed, A.; Mubarak, R.I. High Efficiency Tandem Perovskite/CIGS Solar Cell. In Proceedings of the 2020 2nd International Conference on Smart Power & Internet Energy Systems (SPIES), Bangkok, Thailand, 15–18 September 2020; pp. 224–227. [CrossRef]
- 69. Benaicha, M.; Dehimi, L.; Pezzimenti, F.; Bouzid, F. Simulation analysis of a high efficiency GaInP/Si multijunction solar cell. *J. Semicond.* **2020**, *41*, 032701. [CrossRef]
- 70. Essig, S.; Allebé, C.; Remo, T.; Geisz, J.F.; Steiner, M.A.; Horowitz, K.; Barraud, L.; Ward, J.S.; Schnabel, M.; Descoeudres, A.; et al. Raising the one-sun conversion efficiency of III–V/Si solar cells to 32.8% for two junctions and 35.9% for three junctions. *Nat. Energy* 2017, 2, 17144. [CrossRef]
- Shen, H.; Jacobs, D.A.; Wu, Y.; Duong, T.; Peng, J.; Wen, X.; Fu, X.; Karuturi, S.K.; White, T.P.; Weber, K.; et al. Inverted Hysteresis in CH3NH3PbI3 Solar Cells: Role of Stoichiometry and Band Alignment. *J. Phys. Chem. Lett.* 2017, *8*, 2672–2680. [CrossRef] [PubMed]