

Design and Simulation of ETL-Free Perovskite/Si Tandem Cell With 33% Efficiency

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Abstract: - Multi-junction (tandem) cell using $\text{MAPbI}_{3-x}\text{Cl}_x$ and silicon as absorbers has been designed and simulated in this paper. The thickness of the silicon layer in the bottom cell is 2 μm allowing it to absorb the transmitted spectrum from the perovskite subcell as much as possible. The thickness of the $\text{MAPbI}_{3-x}\text{Cl}_x$ layer is optimized using a proposed algorithm. The output metrics show that the optimum thickness of the $\text{MAPbI}_{3-x}\text{Cl}_x$ layer was 205 nm. The simulation outputs showed that the proposed tandem cell has an efficiency of 33.09% with an open circuit voltage of 1.9 V and a short circuit current of 19.95 mA/cm^2 .

Key-Words: ETL free; High-efficiency; Perovskite; Si; Tandem.

Received: July 26, 2021. Revised: October 16, 2022. Accepted: November 17, 2022. Published: December 31 2022.

1 Introduction

Over the last few years, there has been a high energy demand. According to statistics, fossil fuels have been the primary source of energy consumed until now. In the coming decades, it is estimated that renewable energy sources, particularly solar cells, will be the primary source of energy overtaking fossil fuels. The market for photovoltaics is currently dominated by multi-crystalline and monocrystalline solar cells made of crystallized silicon. Single-junction solar cells made on crystalline silicon now have power conversion efficiencies of about 25%, [1], whereas the perovskite photovoltaics have an average power conversion efficiency of about 26%, [2], many researches show a promising result of up to 30%, [3].

Single-junction solar cells are limited to absorbing most of the incident AM1.5. One solution to this limitation is using two or more subcells, each having a different absorber layer with a different energy gap and able to absorb different parts of the incident light, [4], to build tandem cells.

The design and optimization of a two-subcell multi-junction solar cell are presented in this paper utilizing SCAPS-1D, [5]. The top ($\text{MAPbI}_{3-x}\text{Cl}_x$) subcell (PSC) consists of CuO, perovskite, and transparent conductive oxide. This subcell is designed without the electron transport layer (ETL) as the transparent conductive oxide is highly doped to apply the function of the electron transport layer beside its primary role as a transparent layer, [6], [7], [8], [9]. The bottom subcell consists of Cadmium

sulfide (CdS) and Zinc oxide (ZnO) layers with a silicon (Si) absorber layer.

The ETL-free PSC is used as the top subcell rather than conventional PSC as it exhibits improved efficiency and stability. In addition, to improve the output metrics of the multi-junction cell, the influence of the thickness of the PSC top subcell absorber layers is studied. The overall tandem cell is assumed to be mechanically stacked and equivalent to an ideal monolithic structure, [10], [11], [12].

The remainder of this work is structured as; section 2 shows the structure, and simulation results of the top ETL-free PSC, and introduces the bottom silicon subcell; the algorithm used to obtain the optimum thickness of the top subcell absorber layer thickness to optimize the tandem cell efficiency is given in section 3; section 4 concludes the work.

2 Formulation of Subcells

The designed ETL-free PSC structure is shown in Figure 1 and specifically in Figure 1 (a). The characteristics of the ETL-free PSC with the thickness of the perovskite material are shown in Figure 2. In this design, the transparent conductive oxide (TCO) layer acts as its main function and the ETL function. The simulation materials are mentioned in Table 1, where the simulation is performed using illumination of AM1.5G at a temperature of 300 °K. The results in Figure 2 shows that the short circuit current density (J_{sc}), Power Conversion Efficiency (PCE), and Fill Factor (FF) of the designed tandem cell increase with increasing the perovskite material thickness up to about 800 nm and then saturated. However, increasing the thickness of the perovskite layer will lead to a decreasing the open-circuit voltage (V_{oc}). An essential note that must be taken into consideration is that the implantation of the practical thickness of the absorber layer can not exceed 1000 nm. The designed ETL-free perovskite solar cell shows excellent performance with a high PCE of about 35%. Additionally, the design is simple.

The proposed Si bottom subcell design is illustrated in Figure 1 and specifically Figure 1(b). The J/V characteristics of this subcell are shown in Figure 3. The simulation settings are the same as in the previous simulations. The simulation shows PCE = 16.35% with FF = 79.06 %, V_{oc} = 0.496 V and J_{sc} = 41.65 mA/cm². The parameters used in the simulation are given in Table 2.

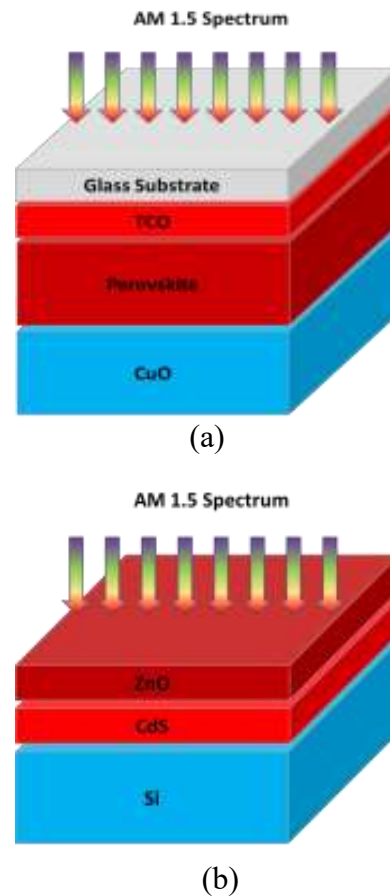


Fig. 1: structure of (a) ETL-free Perovskite subcell; (b) Silicon subcell.

Table 1. Parameters of ETL-free PSC subcell

Parameters		TCO	$MAPbI_{3-x}Cl_x$	CuO
Energy gap (eV)		3.5	1.5, [13]	2.1, [14]
Thickness (nm)		500	variable	400
Relative permittivity		9	6.5, [14]	7.11, [14]
Electron Affinity χ (eV)		4	3.9, [15]	3.2, [14]
Effective density of states (cm ⁻³)	N_C	2.2×10^{18}		
	N_V	1.8×10^{18}		
mobility (cm ² V ⁻¹ s ⁻¹)	μ_e	20	2, [14]	3.4
	μ_p	10	2, [14]	3.4
concentration	N_A (cm ⁻³)	0	0	10^{17}
	N_D (cm ⁻³)	2×10^{19}	10^{18}	0
Density of defects N_t (cm ⁻³)		10^{15} , [16]	10^{10} , [17]	10^{15}

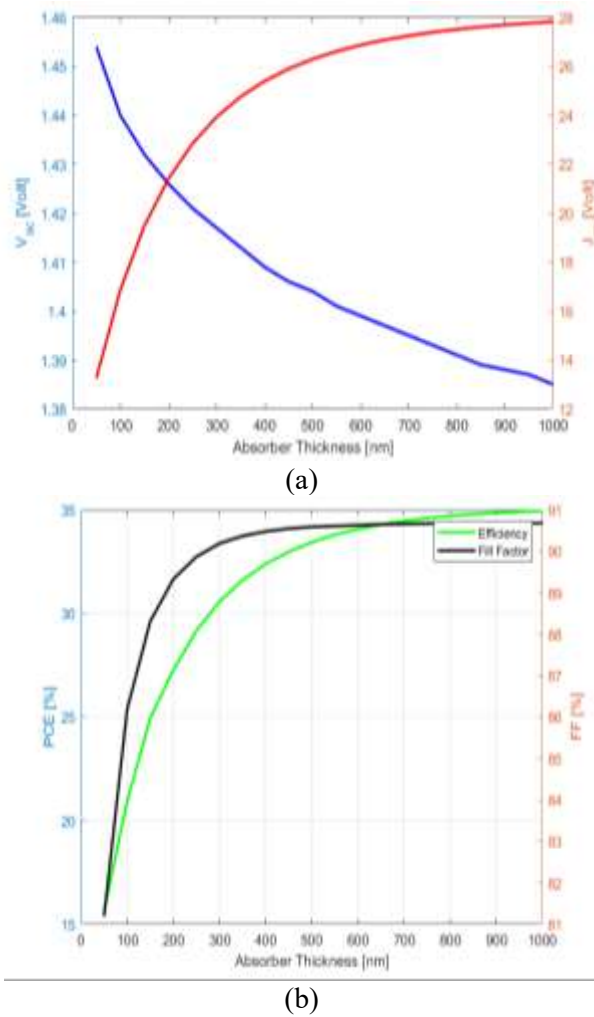


Fig. 2: ETL-free Perovskite subcell characteristics with thickness: (a) V_{oc} and J_{sc} , (b) PCE and FF

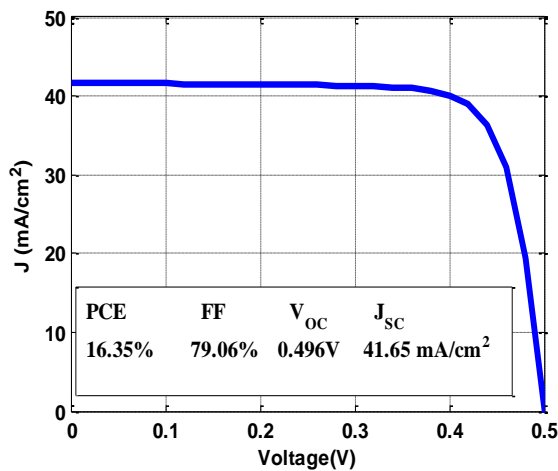


Fig. 3: J/V curve of the Si bottom cell.

Table 2. Parameters of the Si subcell.

Parameters	ZnO	CdS	Si
Energy gap (eV)	3.30, [18]	2.45, [18]	1.12
Thickness (nm)	20	50	2000
Relative permittivity	9.0, [19]	10.0	11.9
Electron Affinity χ (eV)	4.6	4.4	4.05
Effective density of states (cm ⁻³)	N_C	2.2×10^{18}	2.8×10^{19}
	N_V	18×10^{18}	26.5×10^{18}
mobility (cm ² V ⁻¹ s ⁻¹)	μ_e	10^2	1450
	μ_p	25	500
concentration	N_A (cm ⁻³)	-	2×10^{16}
	N_D (cm ⁻³)	10^{20}	0
Density of defects N_t (cm ⁻³)	10^{14}		

3 Multi-Junction Cell

A numerical technique from [20] is used. A two-phase algorithm is employed to optimize the thickness: a course step of 50 nm and a small step of 5 nm. All the junction's performance characteristics are computed based on the resultant thickness at each stage. This algorithm is an improvement of the algorithm from [21]. The modified algorithm is more efficient than the one presented in [21] as the number of overall computations decreases; the suggested modification leads to a faster response for determining the thickness of the top subcell absorber for the 2-terminal multi-junction cell. Furthermore, because the second phase's step size is decreased to 5 nm, it can determine the optimal thickness with higher accuracy (the technique used in [21] has a minimum step size of 10 nm).

ETL-free PSC/Si multi-junction solar cell has a PCE of 33.09% when the perovskite thickness is 205 nm, as illustrated in Figure 4. The multi-junction cell with AM1.5 and filtered AM1.5 are shown in Figure 5.

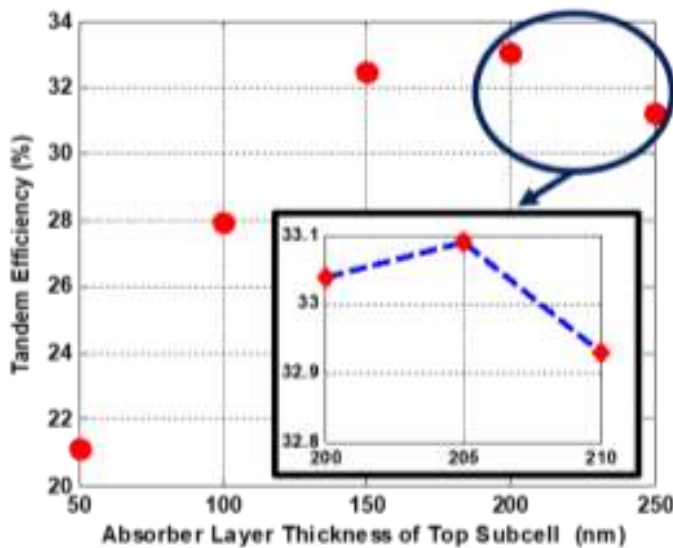


Fig. 4: Tandem cell efficiency of ETL-Free PSC/Si with various thicknesses of the top subcell absorber material.

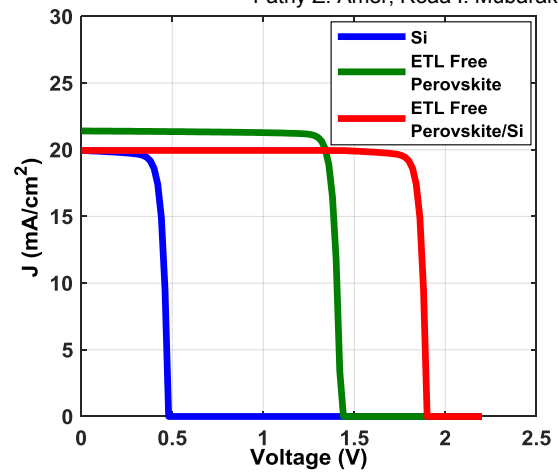


Fig. 6: ETL-Free Perovskite/Si subcells and tandem cell J/V characteristics

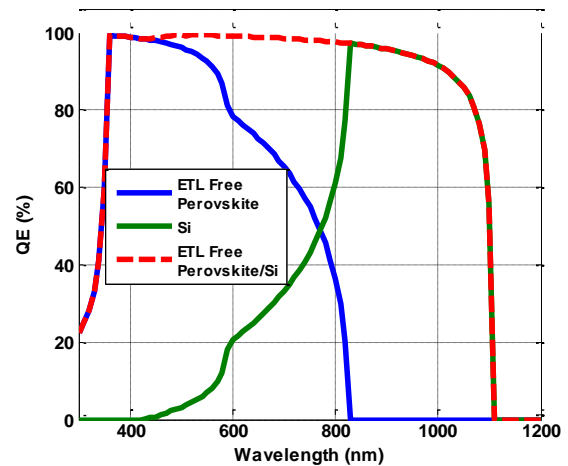


Fig. 7: Quantum Efficiencies of ETL-Free Perovskite/Si subcells and tandem cell.

4 Conclusion

The designed tandem cell has a high-power conversion efficiency and is presented with a practical thickness range. A multi-junction solar cell using perovskite and silicon as absorbers has been presented. An optimization algorithm is presented to optimize the thickness of the perovskite material. The results show that electron transport-layer free perovskite is a promising top sub-cell that can be used with other bottom subcells rather than silicon, the proposed tandem cell has an efficiency of 33.09%

References

- [1] Yoshikawa, Kunta, et al. "Silicon heterojunction solar cell with interdigitated back contacts for a photoconversion efficiency over 26%." *Nature energy* 2017, 2, 17032
- [2] Yang, Woon Seok, et al. "Iodide management in formamidinium-lead-halide-based perovskite layers for efficient solar cells." *Science* 2017, 356, 1376–1379.
- [3] Salah, Mostafa M., et al. "A comprehensive simulation study of hybrid halide perovskite solar cell with copper oxide as HTM." *Semiconductor Science and Technology* 2019, 34, 115009.

Fig. 5: Illumination of the ETL-Free Perovskite/Si tandem solar cell.

The multi-junction overall cell with the highest efficiency has a V_{OC} of 1.9 V, J_{SC} of 19.95 mA/cm², and FF of 87.29% as Figure 6 shows. The Quantum Efficiencies (QEs) of the PSC and Si subcells and the multi-junction cell are shown in Figure 7. At low wavelengths, the QE of the multi-junction cell is almost the same as the used ETL-free perovskite top subcell, while it is about 100% up to the cutoff wavelength (1107 nm) of the bottom subcell.

- [4] Mousa, M., et al. "High efficiency tandem perovskite/CIGS solar cell". *2020 2nd International Conference on Smart Power & Internet Energy Systems (SPIES)*, Bangkok, Thailand, 15–18 September 2020; pp. 224–227.
- [5] Burgelman, M.; et al. "SCAPS Manual"; University of Ghent: Ghent, Belgium, 2016.
- [6] Salah, Mostafa M., et al. "High-Efficiency Electron Transport Layer-Free Perovskite/GeTe Tandem Solar Cell: Numerical Simulation." *Crystals*, 12(7), p.878.
- [7] Salem, Marwa S., et al. "Efficient perovskite solar cell without electron transport layer." *International Journal of Electrical Engineering and Technology*, 34(12), p.1.
- [8] Salah, Mostafa M., et al. "Investigation of Electron Transport Material-Free Perovskite/CIGS Tandem Solar Cell." *Energies*, 15(17), p.6326.
- [9] Basyoni, Marwa Sayed Salem, et al. "On the Investigation of Interface Defects of Solar Cells: Lead-Based vs Lead-Free Perovskite." *IEEE Access*, 9, pp.130221-130232.
- [10] Mousa, Mohamed, et al. "Simulation of High open-circuit voltage Perovskite/CIGS-GeTe tandem cell." *2022 IEEE 49th Photovoltaics Specialists Conference (PVSC)*. IEEE, pp. 1230-1234).
- [11] Madan, Jaya, Rahul Pandey, and Rajnish Sharma. "Device simulation of 17.3% efficient lead-free all-perovskite tandem solar cell." *Solar energy* 2020, 197, 212–221.
- [12] Mousa, Mohamed, et al. "Two-Terminal Perovskite/Silicon Solar Cell: Simulation and Analysis." *2021 3rd Novel Intelligent and Leading Emerging Sciences Conference (NILES)*. IEEE, pp. 409-412.
- [13] Chae, Jungseok, et al. "Chloride incorporation process in CH₃NH₃PbI₃-x Cl x perovskites via nanoscale bandgap maps." *Nano letters* 15, no. 12 (2015): 8114-8121
- [14] Mehra, Rajesh. "Efficient design of perovskite solar cell using mixed halide and copper oxide." *Chinese Physics B* 27, no. 1 (2018): 018801
- [15] Bansal, Shubhra, and Puruswottam Aryal. "Evaluation of new materials for electron and hole transport layers in perovskite-based solar cells through SCAPS-1D simulations." *2016 IEEE 43rd Photovoltaic Specialists Conference (PVSC)*. IEEE, pp. 1-4.
- [16] Salah, Mostafa M., et al. "A comparative study of different ETMs in perovskite solar cell with inorganic copper iodide as HTM." *Optik* 178 (2019): 958-963
- [17] Minemoto, Takashi, and Masashi Murata. "Theoretical analysis on effect of band offsets in perovskite solar cells." *Solar Energy Materials and Solar Cells* 133 (2015): 8-14.
- [18] Wagner, Sigurd, et al. "CuInSe₂/CdS heterojunction photovoltaic detectors." *Applied Physics Letters*, 25(8), 434-435.
- [19] Salah, Mostafa M., et al. "Analysis of an Efficient ZnO/GeTe Solar Cell Using SCAPS-1D." *Proceedings of Seventh International Congress on Information and Communication Technology*. Springer, Singapore, 2023, pp. 677-685.
- [20] Mousa, Mohamed, et al. "Simulation of optimized high-current tandem solar-cells with efficiency beyond 41%." *IEEE Access*, 9, pp.49724-49737.
- [21] Rabady, Rabi Ibrahim, and Hamza Manasreh. "Thicknesses optimization of two-and three-junction photovoltaic cells with matched currents and matched lattice constants." *Solar Energy* 158(2017):20-27.

Conflicts of Interest

The author(s) declare no potential conflicts of interest concerning the research, authorship, or publication of this article.

Contribution of individual authors to the creation of a scientific article (ghostwriting policy)

The author(s) contributed in the present research, at all stages from the formulation of the problem to the final findings and solution.

Sources of funding for research presented in a scientific article or scientific article itself

No funding was received for conducting this study.

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