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Computational Optimization and Parameter Analysis of Perovskite–Silicon Tandem Solar Cells Using SCAPS-1D

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ABSTRACT

The performance of monolithic perovskite/silicon tandem solar cells is strongly influenced by the optical and electrical properties of their constituent layers. In this study, a numerical investigation of a monolithic perovskite/silicon tandem architecture was carried out using SCAPS-1D under standard AM1.5G illumination. The proposed device consists of an FTO/ZnMgO/FA_{0.85}CS_{0.15}Pb(I_{0.6}Br_{0.4})₃/NiCo₂O₄ widebandgap perovskite top sub cell coupled with an ITO/amorphous-silicon/crystalline-silicon heterojunction bottom sub cell. The influence of layer thickness on the photovoltaic response was systematically evaluated by analysing the open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE). ZnMgO and NiCo₂O₄ thicknesses were varied from 10 to 50 nm, while the crystalline-silicon absorber thickness was varied from 50 to 250 nm. Increasing ZnMgO thickness resulted in a gradual PCE improvement from approximately 4.05% to 4.23%, while NiCo₂O₄ produced a comparatively smaller variation. In contrast, silicon thickness had the strongest influence, increasing J_{sc} from 4.71 to 14.68 mA cm⁻² and FF from 79.94% to 82.92%, with the calculated PCE increasing from 2.96% to 9.34%; V_{oc} decreased from approximately 0.79 to 0.77 V. The results demonstrate the competing effects of enhanced optical absorption, carrier extraction, and bulk recombination and provide useful guidelines for thickness optimization of perovskite/silicon tandem structures.

Keywords: SCAPS-1D, Numerical Simulation, Photovoltaic Devices, Tandem Solar cells, Perovskite- Crystalline Silicon Tandem structure

Introduction

The rapid growth of the global population, industrialization, urbanization and digital infrastructure has resulted in an unprecedented increase in worldwide energy demand. Reliable electricity has become indispensable for transportation, communication, healthcare, manufacturing and modern economic development. At the same time, concerns regarding climate change, greenhouse gas emissions and the depletion of fossil-fuel resources have accelerated the transition toward cleaner and more sustainable energy systems. Consequently, renewable energy technologies have become central to national and international strategies aimed at achieving energy security and reducing carbon emissions.

Among the available renewable energy resources, solar energy is regarded as one of the most abundant and universally accessible sources. The amount of solar energy reaching the Earth's surface each year is far greater than the current global energy demand. Continuous reductions in manufacturing costs, improvements in photovoltaic efficiency and supportive government policies have led to the rapid deployment of solar photovoltaic systems across residential, commercial and utility-scale applications. (Victoria et al., 2021)

Presently photovoltaic devices are primarily based on crystalline silicon (c-Si), which dominates the commercial market owing to its high stability, well-established manufacturing infrastructure and long operational lifetime. Continuous improvements in wafer quality, surface passivation and contact engineering have enabled crystalline silicon cells to achieve remarkable efficiencies and it constitutes about 90% market share. (Ballif et al., 2022) However, the performance of c-Si solar cells becomes stagnant with a record efficiency of 26.7% which is near to the theoretical Auger limit of 29.4% (Niewelt et al., 2022) for silicon solar cells. However, further reduction in cost demands a pathway to increase the conversion efficiency, which seems to be a far-fetched objective due to the inherent losses such as thermalization and transparent bandgap, associated with single junction devices. The maximum achievable efficiency of solar cells with a single junction has been constrained to 33%, as stated in the S-Q limit, a mathematical expression given by Hans-Joachim Queisser and William Shockley in 1961 (Shockley and Queisser, 1961), (Peters et al., 2023). This limits maximum output through a single-junction solar cell, as the complete utilization of the sun's spectrum is impossible. Conventional single-junction solar cells suffer from intrinsic energy losses because low-energy photons are not absorbed while excess photon energy is dissipated as heat. (Akhil et al., 2021) These unavoidable losses restrict the theoretical efficiency of single-junction devices and motivate the search for

advanced photovoltaic architectures capable of utilizing the solar spectrum more effectively. Numerous cells with different bandgaps can be stacked together to overcome this drawback. Cells with different bandgaps will help absorb photons from various bands, which results in maximum utilization of the sun spectrum, and sequentially, the output of these cells increases. The resultant device is a tandem device with different bandgap sub cells stacked together to form a tandem configuration (Cheng and Ding, 2021; Raza and Ahmad, 2022). Its architecture consists of mechanically stacked layers integrated monolithically and spectrally split. The above device can be grouped as 2T (two terminals), 3T, and 4T according to how the sub cells are connected, that is, whether they are in series or parallel (Di Carlo Rasi and Janssen, 2019). Apart from increasing efficiency, the tandem devices reduce optical and electrical losses. By systematically choosing effective TCO materials and fine tuning its thickness, it is possible to identify highly efficient tandem cell configurations. (De Vos, 1980)

Considering the current market density for silicon based solar cells, one cannot deplete or replace the existing production line with some other material and technology to enhance the conversion efficiency in the near future. Therefore, to open the window for further developments, researchers coupled the silicon-based photovoltaic technology with other promising semiconducting materials to form the tandem solar cell and to improve the harvesting of electromagnetic spectrum emitting by the Sun. Tandem design concurrently mitigates the thermalization and transparent bandgap loss linked to the bottom and top sub cell, respectively. Further, crystalline silicon tandem solar cells are known to have the potential to surpass the Auger limit of 29.4% for silicon solar cells as well as the SQ limit of 33% for single-junction solar cells.

Initially, III-V compound semiconductors were introduced for silicon-based tandem solar cells. However, elevated manufacturing costs associated with III-V compound-based photovoltaic technology restricted its further development (Essig et al., 2017). Therefore, for the development of silicon tandem solar cells for better performance at a lower price, researchers have utilized hybrid organic-inorganic halide-based perovskite materials for the application as top sub cell (Bobela et al., 2017). In particular, monolithic perovskite/silicon tandem solar cells have emerged as an attractive platform because they combine the excellent optoelectronic properties of metal-halide perovskites with the technological maturity and long-term stability of crystalline silicon (Al-Ashouri et al., 2020; Saif et al., 2023). These characteristics reduce recombination losses and facilitate efficient collection of photogenerated charge carriers. Their bandgap can be tuned over a broad range by varying the halide composition or cation chemistry, allowing the material to be tailored for either single-junction or tandem photovoltaic devices. Such architectures have demonstrated rapid improvements in laboratory efficiency and are widely regarded as strong candidates for next-generation photovoltaic modules. (Ying et al., 2024, Ramadan et al., 2023)

Although perovskite materials have been the center of attention for photovoltaic research, there are some issues to be resolved, such as chemical instability and lead-toxicity. Lead is a material widely used in solar cell applications. Despite it being an excellent material choice for solar cells, it has a detrimental effect on the environment, ecology, and living organisms. As an alternative to lead-based perovskite materials, tin halide perovskites have been considered in numerous studies for their similar properties to lead halide perovskite materials (Gu et al., 2020; Lin et al., 2026). Many researchers have used tin halide perovskites in different tandem cell configurations and investigated both numerically and experimentally (Baranwal and Hayase, 2022). Numerical investigation of the $\text{FA}_{0.85}\text{Cs}_{0.15}\text{Pb}(\text{I}_{0.6}\text{Br}_{0.4})_3/\text{CIGS}$ heterojunction tandem cell configuration demonstrated a 28.7% efficiency. In another numerical study, using the $\text{FA}_{0.85}\text{Cs}_{0.15}\text{Pb}(\text{I}_{0.6}\text{Br}_{0.4})_3/\text{CIGS}$ tandem setup, an efficiency of 38% was achieved. Bi et al. reported a tandem configuration with phenethylammonium iodide (PEAI) with an efficiency of 26.8%. (Bi et al., 2024). However, producing high quality film with stable performance is challenging. Another comprehensive study demonstrated that a $\text{Cs}_{0.05}\text{FA}_{0.79}\text{MA}_{0.16}\text{PbI}_{2.49}\text{Br}_{0.51}$ -based device retained approximately 93% of its initial 21.1% PCE after 1200 hours under 30–60% relative humidity (Cao et al., 2021, Cui et al., 2023, Rahman et al., 2023). Transport layers also play a decisive role in determining the overall efficiency and operational stability of perovskite/silicon tandem solar cells. In addition to facilitating selective carrier extraction, these layers suppress interfacial recombination, improve band alignment and contribute to efficient charge transport. Careful selection of electron and hole transport materials is therefore essential for maximizing photovoltaic performance. (Sudhakaran Menon and Krishnamoorthy, 2026). Thus, Electron transport layers (ETLs) and hole transport layers (HTLs) are essential components of high-efficiency perovskite solar cells.

Device Structure And Modelling

Recent advances in perovskite/silicon tandem photovoltaics have focused on wide-bandgap perovskite absorbers, selective transport layers, interface engineering and optical management (Aydin et al., 2024; Fu et al., 2022a; Shi et al., 2024). Nevertheless, systematic numerical investigations that combine transport-layer optimization, absorber-thickness optimization, spectral filtering and current matching remain important for designing practical tandem architectures. (Singh et al., 2025) In the present work, two sub cells are considered. The top sub cell consists of a front FTO contact, ZnMgO electron transport layer, $\text{FA}_{0.85}\text{Cs}_{0.15}\text{Pb}(\text{I}_{0.6}\text{Br}_{0.4})_3$ perovskite absorber and NiCo_2O_4 hole transport layer. (Eperon et al., 2014; Wang et al., 2022, Yang et al., 2021, Gamal et al., 2021)). The bottom sub cell is based on a crystalline-silicon heterojunction incorporating ITO and amorphous-silicon-based selective layers. (Jošt et al., 2020) The standalone sub cells are first optimized under

the AM1.5G spectrum. The transmitted spectrum from the optimized top cell is then used as the incident spectrum for the bottom cell. (Albrecht et al., 2016). This procedure preserves the spectral interaction between the top and bottom devices and allows the current generated by the two sub cells to be compared on a consistent basis. (Bett et al., 2023) (Aydin et al., 2020). The tandem solar cell's current density is limited by the low short-circuit current (J_{sc}) of the specific sub-cell that connects in series to form the tandem configuration. The final open-circuit voltage (V_{oc}) is obtained by summing up the voltages of both the top and bottom sub-cells at their current matching points. The fill factor (FF) is obtained after calculating the open-circuit voltage (V_{oc}) and short-circuit current (J_{sc}). To calculate the power conversion efficiency (PCE), the ratio of the generated maximum power to the total incident power on the cell is considered. The incident light has an intensity of 1000 W/m^2 and gets identified by its standard AM 1.5G spectrum. ZnMgO is investigated through thickness optimization because its thickness can influence electron extraction, interfacial recombination, optical transmission and the resulting photovoltaic parameters. (Bhattarai et al., 2024) NiCo_2O_4 provides selective hole extraction and contributes to favourable band alignment at the perovskite/HTL interface. (Li et al., 2021; Wang et al., n.d.) The optimized top cell is subsequently coupled to the silicon bottom cell through spectral filtering and current matching. (Liu et al., 2023). In the present study, the thickness of ZnMgO layer and NiCo_2O_4 layer was systematically varied over 10–50 nm, and the resulting changes in V_{oc} , J_{sc} , FF and Efficiency were used to identify its influence on the top-cell performance. Similarly the thickness of the silicon layer in the bottom sub cell consisting of ITO/n-type a-SiO₂:H/i-a-Si:H/n-type c-Si/i-a-Si:H/p-type a-Si:H. was also varied to study the effect on various photovoltaic parameters of the resulting tandem device. The device structure is represented in the corresponding schematic figure (Figure 1)

The top cell filtered spectrum is computed using the following formula to model the tandem device:

$$S(\lambda) = S_{i(\lambda)} \cdot \exp\left(\sum_{i=1}^n -\alpha_i(\lambda)d_i\right)$$

where $S_f(\lambda)$ is the filtered spectrum light intensity from the top sub-cell, $S_i(\lambda)$ is the incoming standard AM1.5G spectrum light intensity (W/m^2), α_i is the corresponding material's absorption coefficient, and d_i is the thickness. The subscript i represents materials ($i = 1, 2, 3$, and 4) for TCO, ETL, perovskite absorber, and HTL materials, respectively (Islam et al., 2021). The SCAPS Layer Properties panel provided access to each material's absorption coefficients (Alonso-Álvarez et al., 2018). The bandgap energy determines the absorption edge, while the magnitude and spectral dependence of the absorption coefficient are governed by the electronic structure and optical transitions of the material. (Chen et al., 2020)

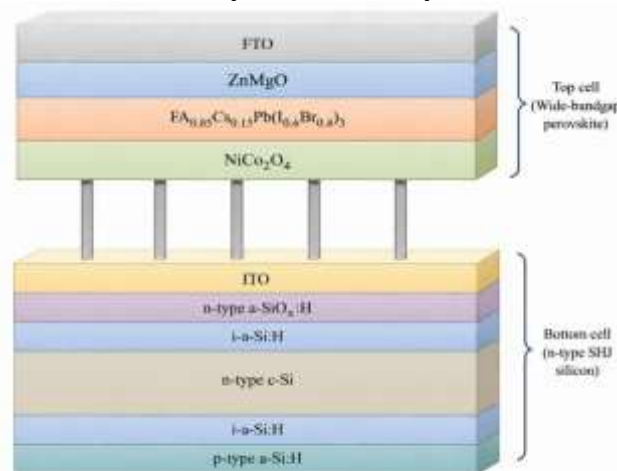


Figure 1: Schematic diagram of the proposed device structure

Parameters Of Simulation

The electrical and optical parameters used for the SCAPS-1D simulations were collected from the literature and from the parameter set adopted for the present device model. The simulated materials are FTO, ZnMgO, $\text{FA}_{0.85}\text{Cs}_{0.15}\text{Pb}(\text{I}_{0.6}\text{Br}_{0.4})_3$, NiCo_2O_4 , ITO, n-type a-SiO₂:H, i-a-Si:H, n-type crystalline silicon and p-type aSi:H. The thickness of the layers was optimized where required for the standalone and tandem simulations. Defect distributions and recombination parameters are applied consistently according to the selected SCAPS parameter set. Table 1 summarizes the key parameters adopted for the individual layers of the proposed device and Table 2 gives the interfacial defect parameters.

Table 1: The different material and their parameters used in the simulation

Layer	FTO	ZnMgO	$\text{FA}_{0.85}\text{Cs}_{0.15}\text{Pb}(\text{I}_{0.6}\text{Br}_{0.4})_3$	NiCo_2O_4	ITO	n-type aSiOx: H	i-a-Si:H	n-type c-Si	i-a-Si:H	p-type a-Si:H
Thickness (nm)	200	50	400	30	25	75	5	180	5	5
Eg (eV)	3.20	3.50	1.79	2.30	3.72	1.40	1.72	1.12	1.72	1.72
Electron affinity χ (eV)	4.40	3.95	3.90	3.48	3.60	3.94	3.80	4.05	3.80	3.80
ϵ_r	9.0	10.0	25.0	11.9	9.4	11.9	11.9	11.9	11.9	11.9
Nc (cm^{-3})	2.2×10^{18}	4.0×10^{18}	2.2×10^{18}	2.0×10^{21}	2.2×10^{19}	2.8×10^{19}	2.5×10^{20}	2.8×10^{19}	2.5×10^{20}	2.5×10^{20}
Nv (cm^{-3})	1.8×10^{19}	9.0×10^{18}	1.8×10^{19}	2.0×10^{21}	1.8×10^{19}	1.4×10^{19}	2.5×10^{20}	1.04×10^{19}	2.5×10^{20}	2.5×10^{20}
μ_n (cm^2/Vs)	90	50	20	1	10	1400	20	1400	20	20
μ_p (cm^2/Vs)	90	20	20	40	10	450	5	450	5	5
v_n (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	2×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
v_p (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	2×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
ND (cm^{-3})	2×10^{19}	1×10^{17}	0	0	1×10^{19}	1×10^{20}	0	5×10^{16}	0	0
NA (cm^{-3})	0	0	1×10^{14}	1×10^{18}	0	0	0	0	0	1×10^{20}
Nt (cm^{-3})	1×10^{15}	1×10^{15}	1×10^{14}	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{16}	1×10^{15}	1×10^{16}	1×10^{15}
Reference	Singh et al.	Nur-E-Alam et al. (2025).	[Nikfar & Memarian (2022)] Burwell et al.]	Islam et al. (	[Singh et al.,R2]	Singh et al.	Singh et al.,R2]	Singh et al.	Singh et al.,R2]	Singh et al.,R2]

Table 2: The different interfacial parameters of the device

Interface	ZnMgO / perovskite	Perovskite / NiCo_2O_4	i-a-Si:H / n-c-Si	n-c-Si / i-a-Si:H	i-a-Si:H / p-a-Si:H
Defect type	Neutral	Neutral	Neutral	Neutral	Neutral
σ_n (cm^2)	1×10^{-17}	1×10^{-17}	1×10^{-15}	1×10^{-15}	1×10^{-19}
σ_p (cm^2)	1×10^{-18}	1×10^{-18}	1×10^{-15}	1×10^{-15}	1×10^{-19}
Distribution	Single	Single	Single	Single	Single
Energy level	0.60 eV above VB	0.60 eV above VB	0.60 eV	0.60 eV	0.60 eV
Nt (cm^{-2})	1×10^{10}	1×10^{10}	1×10^{10}	1×10^{10}	1×10^{10}

Results And Discussion

(a) Effect of ZnMgO Thickness

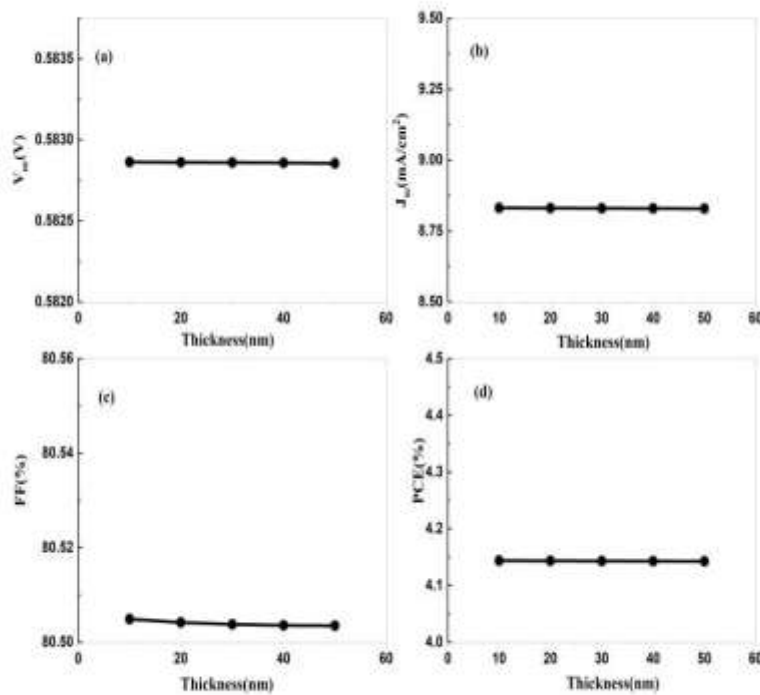


Figure 2. Effect on the thickness of ETL layer on the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and the efficiency.

Increasing the ZnMgO thickness from 10 nm to 50 nm produced a gradual improvement in V_{oc} and J_{sc} , while the FF remained nearly constant at approximately 80.5% as shown in Figure 2. Consequently, the PCE increased from approximately 4.05% at the lower thickness to approximately 4.23% at the upper end of the investigated range. The relatively small variation in FF indicates that the principal improvement arises from changes in carrier extraction and photocurrent generation rather than a major modification of the resistive losses. These results demonstrate that ZnMgO thickness is an important design parameter for the proposed FTO/ZnMgO/ $FA_{0.85}Cs_{0.15}Pb(I_{0.6}Br_{0.4})_3/NiCo_2O_4$ top cell. Within the investigated range, the 50 nm ZnMgO layer gives the highest simulated PCE and is therefore selected as the preferred thickness for subsequent tandem modelling, subject to consistency with the final current-matching configuration.

(b) Effect of Crystalline-Silicon Thickness

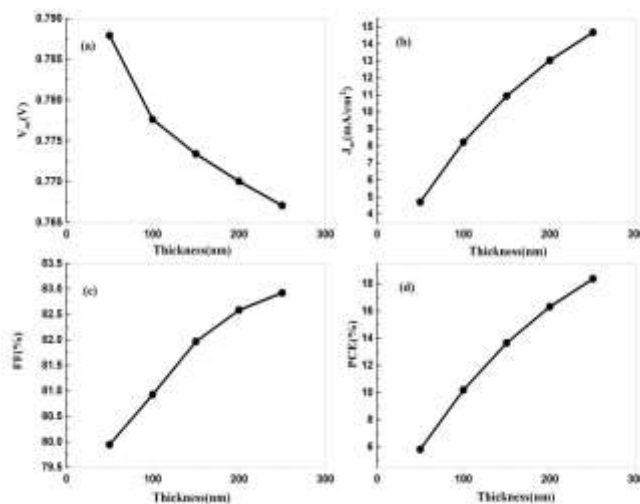


Figure 3. Effect on the thickness of Silicon Absorber layer on the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and the efficiency.

As clearly indicated by Figure 3, the crystalline-silicon absorber exhibited the strongest thickness dependence among the investigated layers. Increasing the absorber thickness from 50 nm to 250 nm resulted in a decrease in V_{oc} from 0.79 to 0.77 V, while J_{sc} increased substantially from 4.71 mA cm^{-2} to 14.68 mA cm^{-2} . The FF simultaneously increased from 79.94% to 82.92%. Consequently, the calculated PCE increased progressively from approximately 2.96% to 9.34%. The pronounced increase in J_{sc} demonstrates the importance of absorber thickness for improving the utilization of long-wavelength photons transmitted through the wide-bandgap perovskite top cell. The accompanying reduction in V_{oc} indicates the competing influence of increased bulk recombination at larger absorber thicknesses.

(c) Effect of NiCo_2O_4 Thickness

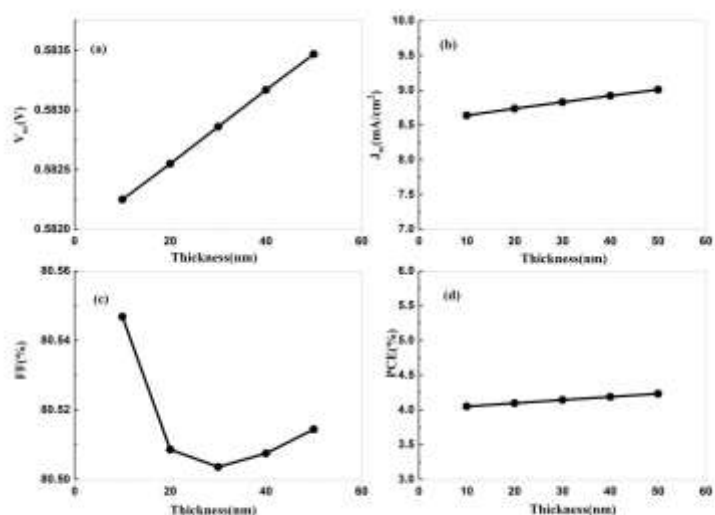


Figure 4. Effect on the thickness of HTL layer on the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and the efficiency.

A comparatively smaller thickness dependence was observed for the NiCo_2O_4 hole transport layer. Increasing its thickness from 10 nm to 50 nm resulted in a slight increase in V_{oc} and J_{sc} , whereas the FF remained close to 80.5% with only minor variation. The corresponding PCE increased gradually across the investigated range, reaching approximately 4.23% at 50 nm. Thus, NiCo_2O_4 thickness provides an additional parameter for optimizing selective hole transport in the proposed top sub cell. The variation of various photovoltaic parameters as represented in Figure 4.

Conclusion

In this work, a monolithic perovskite/silicon tandem solar cell comprising $\text{FTO/ZnMgO/FA}_{0.85}\text{Cs}_{0.15}\text{Pb}(\text{I}_{0.6}\text{Br}_{0.4})_3/\text{NiCo}_2\text{O}_4$ as the top sub cell and an $\text{ITO/amorphous silicon/crystalline-silicon}$ heterojunction as the bottom sub cell was numerically investigated using SCAPS1D. The results show that layer thickness strongly influences device performance through the combined effects of carrier extraction, optical absorption, and recombination. For the ZnMgO , increasing thickness from 10 to 50 nm gradually improves V_{oc} and J_{sc} , while FF remains nearly constant at ~80.5%, resulting in a PCE increase from ~4.05% to 4.23%. This improvement is mainly associated with enhanced electron extraction and photocurrent generation without significant additional resistive loss. The NiCo_2O_4 shows a comparatively weaker dependence, with increasing thickness from 10 to 50 nm slightly improving V_{oc} and J_{sc} , while FF remains close to 80.5%; consequently, PCE increases gradually to ~4.23%, indicating improved hole extraction and interfacial transport. The crystalline-silicon absorber exhibits the strongest thickness dependence. Increasing its thickness from 50 to 250 nm increases J_{sc} from 4.71 to 14.68 mA cm^{-2} and FF from 79.94% to 82.92%, while V_{oc} decreases from ~0.79 to ~0.77 V. The resulting PCE increases from ~2.96% to 9.34%. The strong increase in J_{sc} results from enhanced absorption of long-wavelength photons transmitted through the wide-bandgap perovskite top cell, whereas the reduction in V_{oc} is associated with increased bulk recombination at larger absorber thicknesses. Thus, absorber thickness has the greatest influence among the investigated layers. Overall, the results demonstrate that optimal device performance requires a balance between optical absorption, carrier extraction and recombination rather than maximizing any single parameter. Future studies should focus on tandem current matching, interface-defect and doping optimization, advanced optical management, temperature-dependent modelling and experimental validation.

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