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Performance assessment of an eco-friendly tandem solar cell based on double perovskite $Cs₂AgBiBr₆$

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ABSTRACT

Tandem solar cells have a wider photon absorption range, allowing them to provide better efficiency than singlejunction SC. The upper cell absorbs high-energy photons, while the lower cell absorbs low-energy filtered photons. However, in order to obtain affordable, efficient, and long-lasting SC, the absorber layers of the *top* and *bottom* cells must be integrated with an adequate bandgap. This research suggests tandem perovskite solar cells as upper band active materials in this setting. The Si homojunction solar cell's performance was improved by investigating the thicknesses of the *p* − *type* and *n* − *type* layers, doping concentrations, and defect densities. The thickness variation of the *perovskite* solar cell (100 − 400 *nm*) is then optimized. To precisely replicate the tandem devices, the estimated spectra of the perovskite SC are optically filtered onto the lower cells. Current matching was achieved by adjusting the thickness of the *perovskite* sub-cell with different bottom layer thicknesses, and the optimized efficiency of 36*.*26% for the *perovskite/Si* tandem device was shown. The discoveries will open the door for the upcoming creation of *high* − *efficiency*, low-energy solar cells.

> solar cells, a variety of materials are utilized as absorbers. According to the absorber material used, solar cells are divided into generations, with organic solar cells being the third generation [\[2](#page-8-0)–4]. Other uses for perovskite include a wide range of industries. The first are pricey solar cells made solely of silicon. Low-cost amorphous *Si* solar cells are the second type. The third generation, which has cheap costs, is also being developed; it is highly PCE stabilized. Quantum Dots in applications including photodetectors, Perovskite Solar Cells, and most recently Liang et al. They created high-performance photodetectors using this discovery after successfully fabricating a number of perovskite films [[5](#page-8-0)]. Formula: *ABX*3 (*A* = monovalent organic/inorganic cation, *B* = divalent metal, and $X = anion$ (*I, Br, Cl, F)*) describes organic-inorganic halide perovskites. Pb toxicity, repeatability, and device stability are still serious issues even when the PCE is higher than 25 % [\[6,7\]](#page-8-0). Lead-free double halide perovskites with the formula A2BCX6 have exceptional optoelectronic capabilities that are well-recognized in the field of

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1. Introduction

The world is moving away from energy conversion methods based on fossil fuels and toward clean, *renewable* energy [\[1\]](#page-8-0). Production of SC typically rises twice a year. In order to absorb the sunlight that enters

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photovoltaics $[8,9]$ $[8,9]$ $[8,9]$ $[8,9]$ $[8,9]$. They can be thought of as a potential replacement for Pb-based *perovskites* due to their exceptional environmental stability, appealing optoelectronic properties, and low toxicity [[10,11](#page-8-0)]. The development of undesired phases makes HDP (halide double perovskites) synthesis difficult. Recently produced compounds include $Cs₂NaBiI₆$ [[12\]](#page-8-0), $Cs₂AgInCl₆$ [[13,14](#page-8-0)], $Cs₂AgSbCl₆$ [[15\]](#page-8-0), and $Cs₂AgBiX₆$ $(X = Br, Cl)$ [\[16](#page-8-0),[17\]](#page-8-0). Cs₂AgBiBr₆ is a good prospective replacement for Pb-based perovskites because of its nontoxicity and remarkable properties appropriate for PSCs. However, the $Cs₂AgBiBr₆ HDPs still exhibit$ significant limitations, including a broad interdite indirect band, a strong *electron* − *phonon* couplage, and dominant surface defects [\[11](#page-8-0)]. Greul et al. already built the device configuration $FTO/c-TiO₂/m-$ TiO₂/Cs₂AgBiBr₆/spiro-OMeTAD/Auutilizing the solution process approach, with a *PCE* of 2*.*43% [[18\]](#page-8-0). An antisolvent solution procedure was previously used to construct a $Cs₂AgBiBr₆$ -based SC with a PCE of 1.26 % (*FTO*/c-TiO₂/m TiO₂/Cs₂AgBiBr₆/ *PTAA*/*Au*) [[19\]](#page-8-0). Furthermore, a Cs₂AgBiBr₆-based SC (*ITO/ SnO*₂/Cs₂AgBr₆/ *P3HT*/ *Au*) with 1.44 % efficiency was developed using the low-pressure aided solution approach [[20\]](#page-8-0). *Zhao et al.* developed a device based on a thin Cs₂Ag-BiBr6 film with an *ITO*/ *SnO*2/Cs2AgBiBr6/ *SpiroOMeTAD*/Au structure (average grain size of around 500 *nm*) [\[21](#page-8-0)].

Our goal is to model the multijunction device with *perovskite* substrate (both top and bottom cell) while focusing on various difficulties and options [\[22](#page-9-0)]. Additionally, a tandem *SC* with a rigid terminal was made available for the first time. Its open-circuit voltage (*Voc*) was about 1*.*7 *V*, and its power conversion efficiency was approximately 18% [\[23](#page-9-0)]. Additionally, this research endeavor demonstrates an increase in efficiency of over 30 %. The findings are achieved through in-depth analysis, simulation, and computation on a variety of configurations, which can help to improve the results and performance even more. In order to simulate, calibrate, and test tandem combinations of upper and lower perovskite solar cells, the work has been broadened. We also took into account other sociological and environmental issues, thus in order to lessen their impact, we used a lead-free perovskite as the top cell. This design can produce results that are advantageous in terms of both economics and power conversion efficiency [\[24](#page-9-0)].

We studied the potential benefits of implementing the material $Cs₂AgBiBr₆$ as an absorber in tandem SC to improve energy conversion efficiency in this paper. To that purpose, DFT calculations were utilized to explore the electrical and optical properties of $Cs₂AgBiBr₆ [25]$ $Cs₂AgBiBr₆ [25]$, and the SCAPS software was also used to do numerical simulations of the material's application in SCs. The approach and computational specifics are described in the first section. The second section, which similarly summarizes and discusses our findings, goes into detail on the application of the researched material in solar cells.

In this situation, we established a novel device with an ITO/ZnSe/ $Cs₂AgBiBr₆ structure that made use of several ETM/HTM. We improved$ both their doping densities and thicknesses, and we looked into the effects of the thickness of the absorber, its flaws, and the time and

resources needed. Some of the input factors that we examined in terms of how they affected the performance of our device included the defect density at the *HTL/Cs*₂AgBiBr₆ and Cs₂AgBiBr₆/ *ETL* interfaces, the electrical affinity of the *ETL*, and the work function of the front/back contact.

2. Device design and numerical simulation

2.1. Simulations and the suggested device's architecture

In the present study, the numerical solution is carried out utilizing the *SCAPS* − 1*D* simulation tool [\[26](#page-9-0)–29]. The Ghent University developed SCAPS, which simulates photovoltaic devices by resolving fundamental semiconductor equations like the Poison equation and the continuity equations for electrons and holes. It is an effective modeling tool that simulates electronics with up to seven separate semiconductor layers, each with a distinct set of interface and ground faults. The top *perovskite* cell (TP) is first simulated, yielding a PCE of approximately 18.61 %. The bottom silicon-based cell (BC) is then simulated, yielding a PCE of 22.77 %. This method of individual simulation is known as a stand-alone configuration. Furthermore, the simulation is run on multiple spectra and absorber layer thicknesses to determine the present matching condition. The architecture of the top and bottom cells of the structure under study are depicted in [Fig. 1](#page-4-0)(a). In order to solve our problem numerically, we employed the following three equations: (1) *Poisson*′ *s equation*, (2)*/*(3) continuity equations for *electrons/holes*, and power conversion efficiency (*PCE*) [[30,31\]](#page-9-0) are used to calculate performance indicators such as *FF*, Jsc, *Voc,* and *PCE.*.

$$
-\frac{d}{dx}\left(\varepsilon(x)\frac{d\psi}{dx}\right) = q\left[p(x) - n(x) + N_d^+(x) - N_a^-(x)\right]
$$
\n(1)

$$
\frac{\partial j_n}{\partial x} = q\left(R_n - G + \frac{\partial n}{\partial t}\right) \tag{2}
$$

$$
\frac{\partial j_p}{\partial x} = q \left(R_n - G + \frac{\partial p}{\partial t} \right) \tag{3}
$$

n/p: *Total electron/hole density*.

N⁺ *^d* / *N*[−] *^a* : *Ionized donor/acceptor*− *like doping concentration*.

jn/ *jp*: *Electron/hole current density*.

Rn/ *Rp*: *Electron/hole recombination rates.*.

ψ, ε, G, and q: The *electrostatic potential*, *permittivity*, *generation rate*, and *electron charge* respectively.

[Table 1](#page-4-0) lists all the simulated materials' specific electrical properties. The equivalent circuit is used to create the *J* − *V* curve of the tandem solar cell from those of each sub-cell in order to create a clone of the tandem device. We have made the assumption that the tunnel junction is perfect, with no optical or electrical loss occurring between the two subcells.

Fig. 1. A cross-sectional illustration of (a) a *BSC* stand-alone bottom cell and (b) an all-perovskite *TSC*, where the typical *AM*1*.*5 spectrum illuminates the *TC* and the filtered *TC* spectrum is sent to the *BC* for full device simulations.

An optical transmission filter defined by equation [\(1\)](#page-3-0) is defined on top of the front contact and illuminates the wide bandgap sub-cell with the standard *AM*1*.*5 *G spectrum*, while the lower narrow bandgap cell is illuminated by a *filtered spectrum* that mimics the optical properties of the *top cell* [[32\]](#page-9-0). Thin-film interference-related reflection losses are not included in this computation. Fig. 1 shows the optical filters made for *perovskite* SC with various band gaps and thicknesses, whereas [Fig. 2](#page-5-0) shows the absorption coefficients of each layer in *eq*.

[Fig. 2](#page-5-0) b) depicts the power density of the spectral lines from the 1.5G source, as well as the energy attained by photons entering the cell after passing through different layers of the absorbent $Cs₂AgBiBr₆$ layer. As

Table 1

Parameters used in the device simulation for every layer.

the absorber's thickness grows, so does its power. According to [Fig. 2](#page-5-0) b), as the absorber layer with a high band gap thickens, the optical transmission decreases, lowering the Jsc of the lower cellule and limiting the amount of light that can elucidate it. To find the best combination of these characteristics, we investigated how the thickness of the Cs2Ag-BiBr6 layer affects the photovoltaic properties of two sub-cells. To do this, we used a filtered spectrum calculated with varying absorber film sizes in the upper cellule.

$$
S(\lambda) = S_0(\lambda) \left(\exp(\alpha_{ITO}.d_{ITO}) \exp(\alpha_{ZnSe}.d_{ZnSe}) \exp(\alpha_{Cs_2AgBiBr_6}.d_{Cs_2AgBiBr_6} \right) \tag{4}
$$

Where:

 $\alpha(\lambda)$: *Absorption coefficient, d: Thickness of a layer,* $S_0(\lambda)$ *: <i>AM* 1*.5G spectrum, S*(*λ*): *Filtred spectrum by top cell*,

2.2. *Analysis and calibration of a perovskite-based cell (Eg = 1.16 eV) in stand-alone configuration*

The aim here is to achieve material savings by reducing the thickness of the $Cs₂AgBiBr₆$ absorber. To achieve this, we carried out a study to optimise the thickness of $Cs₂AgBiBr₆$ while varying its thickness from 0.25 μm to 2 μm. The effect of this adjustment on the suggested solar cell's photovoltaic performance was further researched. First, the upper cell's calibration was performed, and the cell's perovskite thickness was set at 2 μm. The upper cell contained perovskite with a bandgap of 1.417 eV. It can be shown that the two major characteristics of the SC (*PCE* and *Jsc*) grow, then peak at 1*.*25 *μm* before declining somewhat for $Cs₂AgBiBr₆ thickness values between 1.25 μ m and 3 μ m. It reaches a$ maximum for the *FF* form factor at a thickness of 1*.*25 *μm* and then drops significantly. Based on this result, we may estimate that the optimal thickness of the Cs₂AgBiBr₆ absorber is 1.25μm. The open-circuit voltage *Voc* drops with increasing absorber thickness while remaining high.

The matching *J* − *V* and *QE* curves depicted in [Fig. 3\(](#page-5-0)a and b) a thorough examination of $Fig. 3(a)$ $Fig. 3(a)$ reveals that raising the perovskite thickness increases the J_{SC} while decreasing cell efficiency. The J_{SC} rises dramatically while the cell V_{oc} stays constant. J_{SC} increases with increasing perovskite thickness because photon absorption increases in the thicker perovskite layer. The rate of electron-hole pair formation rises as a result of the higher cumulative absorption, raising the likelihood of collection and consequently the *Jsc*.

Furthermore, the *top* and *bottom* cells' quantum efficiency [\[33](#page-9-0)] is assessed. The quantity of current generated by a solar cell when exposed to photons of a particular wavelength is known as quantum efficiency, which is a crucial solar cell property. [Fig. 3](#page-5-0) (b) depicts the top and bottom cells' quantum efficiency at varying incoming wavelengths. We found that the highest QE response for the perovskite layer is recorded in the 80–90 % range between 350 and 900 nm, whereas this range is located beyond 1000 nm for Si. This is also visible in [Fig. 3](#page-5-0) (b), where the

Fig. 2. Absorption coefficient of each ayer in the TSC and the Optical Power Density of the Absorber layer.

Fig. 3. (a) *J* − *V curve*, (b) *external QE* for *perovskite* (*top cell*)*, Si* (*bottom cell*)*.*.

drop in QE is caused by insufficient light absorption in the thinner perovskite layers. According to the QE diagram of two subcells, the higher cells absorb most of the photon energy at shorter wavelengths. The closeness of the QE between the simulated and experimental operations confirms the simulation design, it should be underlined. After calibration of the sub cells (Top and Bottom) we opted for many values of the most important parameters controlling the solar cells functioning. Table 2 below show a summary of the inputs used for each sub cell in the final stage of the simulation study.

2.3. Effect of charge carrier density and Cs2AgBiBr6 absorber layer thickness

How to create environmentally friendly solar cells with a high (%) using incredibly thin absorber layers is the problem facing solar energy experts [[34\]](#page-9-0). Optimal cell performance is achieved by adjusting the absorber layer carrier concentration and thickness, which have a considerable impact on the structural design of solar cells. [Fig. 4](#page-6-0) illustrates how concentration and thickness affect the photovoltaic performance of the proposed solar cell. The concentration and thickness of the

Table 2

The photovoltaic properties of the optimized *perovskite* (*top cell*) solar sell and, *Si* (*bottom cell*) solar sell.

Cell type	$V_{ac}(V)$	$J_{sc}(mA/cm^2)$	$\boldsymbol{FF}\ (\%)$	PCE(%)
Si (Optimal condition)	0.75	34.39	85.47	22.28
$Cs2AgBiBr6$ (Optimal condition)	1.01	27.90	86.45	24.44

Cs₂AgBiBr₆-based absorber layer were altered between $10^{13} \rightarrow 10^{18}$ cm^{-3} and 0.2 μ *m* → 2 μ *m*, respectively, in order to investigate the cell's performance. The thickness of the $Cs₂AgBiBr₆$ absorber layer is shown in [Fig. 4](#page-6-0) to be an essential parameter for cell performance. The efficiency of the cell's energy conversion can be decreased by adjusting the thickness of this layer. V_{oc} increases a little bit as the $Cs_2AgBiBr_6$ absorber layer's thickness and concentration rise. J_{sc} increases from 8.50 \rightarrow 30.20 $mA/cm²$ when absorber layer thickness increases between 0.2 μ m and 2 μm, owing to enhanced absorption of longer wavelength photons in this layer, which is similar with the findings of [[35,36\]](#page-9-0). The maximal *Jsc* contour zone does expand into the area of greater thickness, but the concentration of acceptors continues to be largely independent of the absorption layer on the other hand.

As a result, J_{sc} decreased marginally. Due to an increase in the device's series resistance, the form factor (*FF*) drastically dropped as the $Cs₂AgBiBr₆ thickness grew. The simulated device can have a η (%) > 22$ % with a concentration ranging from $10^{16} \rightarrow 10^{18} \text{cm}^{-3}$ and a thickness *>*1.45 μm (see [Fig. 4](#page-6-0)). A maximum *PCE* (%) of 22*.*2% was discovered in this study at a user concentration of 10^{18} cm^{-3} and an absorber layer thickness of 2 *μm*. An increase in the absorber layer carrier concentration (Cs₂AgBiBr₆ > 10^{17} cm⁻³) has a negative effect on device performance (increase in Auger recombination).

The FF of the SC increased from 88.60 % for the absorber layer cell. This increase can be interpreted as a larger rise in the maximum power output of the solar cell with the *ITO*/ZnSe/Cs₂AgBiBr₆ configuration. This increase in maximum power is due to the use of absorber perovskite, which reduces charge carrier recombination losses on the rear side, as seen by the *quantum efficiency* curves (see Fig. 3-b). These

Fig. 4. The contour figure shows how the performance of SC is affected by variation of thickness and carrier concentration of the Cs₂AgBiBr₆ absorber layer.

enhancements have led to a notable increase in the *PCE* of the cell, going from 18.06% for the cell without the $Cs₂AgBiBr₆$ layer to 22.20% for the cell with the latter layer inserted due to the stability and good charge carrier generation provided by the latter layer. It should be noted that when the cells are stacked in tandem, the yield improves to approximately 36.26 %.

2.4. Cs2AgBiBr6/Si tandem solar cell

The top and bottom cells of the tandem device must have an equal current density. The two solar cells in 2 − *T monolithic* tandem devices work as two diodes in series [\[37](#page-9-0)]. Thus, the SC that generates the lower current limits the overall current of the tandem device, and the voltage is equal to the sum of the voltages of the upper and lower cells. The bandgap and thickness of the *perovskite* SC were shown to directly affect its J_{sc} in the preceding section. Equation (1) states that when the wide-bandgap absorber layer's thickness increases, optical transmission decreases, lowering the light power impinge on the lower cell and, consequently, the lower cell's *Jsc*. In order to determine the ideal mix of these elements, we investigated the effects of perovskite layer thickness, electron and hole concentrations, and photovoltaic properties of the tandem solar cell. A single filtered transmitted spectrum was produced and utilized to irradiate the lower cell for each top absorber layer thickness that was chosen.

As shown in [Fig. 5](#page-7-0), for low absorber thicknesses in the higher cell, the current generated diminishes, limiting the tandem device's total J_{SC} . The J_{sc} expands as the perovskite absorber's thickness rises, but it also prevents the top cell's optical transmission, limiting the bottom cell's $J_{\rm sc}$ c. As a result, the *Jsc* of the *bottom cell* serves as a limiting factor for the overall *Jsc* once the optimal thickness point is achieved, and the PCE decreases. The optical absorption edge of the *perovskite* layer has a blue shift, which causes the ideal thickness point to change when the bandgap varies. The bandgap and thickness of the perovskite layer, which are 1*.*417 *eV* and 400 *nm*, respectively, are combined to create the optimal *PCE* of 23.9%. [Fig. 5](#page-7-0) also illustrates that the J_{sc} is the most important component in tandem device performance and that the *Voc* and *FF* have little influence on the overall *PCE*. The *Jsc* grows with thickness, as shown in the picture, and the point of intersection between the upper and lower cell curves is the ideal place that establishes the optimal conditions for having a tandem cell with improved features. The point of intersection, as indicated in the picture, implies a current of the order of 24.89 mA/cm² with a cell thickness of 400 nm. The bandgap in the higher cell produces a huge V_{oc} of the tandem device, up to almost 1V, as is to be expected. Variations in thickness cause a minor increase in *Voc*, however the impact of thickness is minimal. The fill factor drops in all bandwidths until it reaches the maximum J_{sc} thickness, at which point a trade-off occurs. Solar cells in tandem commonly exhibit this pattern [38–[43\]](#page-9-0).

[Fig. 6](#page-7-0) shows the simulated current-voltage characteristics of a tandem perovskite/Si solar cell, a bottom filtered Si cell, and an upper perovskite cell with a bandgap of 1*.*417 *eV* and a thickness of 400 *nm*. As seen in [Fig. 6,](#page-7-0) the *top* and *bottom* cells' short-circuit currents have excellent current matching and are in a similar range. The majority of photon energy is absorbed by the Si sub-cell at long wavelengths, while the perovskite sub-cell mostly does so at short wavelengths, which explains this pattern. [Table 3](#page-7-0) provides a summary of the photovoltaic characteristics of the simulated 36.26 % tandem solar cell $(Cs_2AgBiBr_6/$ c-Si). [Table 3](#page-7-0) and [Fig. 6](#page-7-0) show that the bottom sub-cell, whose V_{oc} is

Fig. 5. V_{oc} a), J_{sc} b), *FF* c), and *PCE* d) of the simulated *tandem* SC by variation of thickness of Cs₂AgBiBr₆ *perovskite* absorber.

Fig. 6. *J* − *V curve* for *perovskite* top cell, *Si* bottom cell, and *perovskite/ Si tandem* cell.

equal to the sum of the *Voc* of the two sub-cells, restricts the tandem SC's overall *Jsc*.

[Table 4](#page-8-0) evaluates the photovoltaic properties of the current work to those of previously published tandem perovskite solar cells. Our findings suggest that it is theoretically conceivable to obtain more than 36 % PCE in *perovskite/homojunction* tandem solar cells; nonetheless, significant challenges remain. Perovskite solar cells have previously attained efficiencies in excess of 25 %, but due to the existing constraints of manufactured Si solar cells, highly efficient perovskite solar cells and highly efficient perovskite/Si tandem devices are not achievable. We demonstrated that by producing highly doped Si layers with a low defect density and a good *p* − *n* junction interface (injecting perovskite-based absorber layers), we can improve the performance of Si solar cells.

3. Conclusion

We examined a perovskite/Si tandem solar cell with a PCE of approximately 36.28 % using SCAPS-1D software. Separate numerical simulations of the two solar sub-cells were explored. While the bottom cell first used a spectrum filtered by the top cell, the higher cell was lighted with the *AM* 1*.*5 *G spectrum*, followed by investigation of the upper perovskites (1*.*417 *eV*). Then, the absorber layer thickness (20–400 *nm*) and charge carrier density of the two sub-cells were adjusted. In order to match the ideal current, which is achieved by

Table 3 The photovoltaic properties of the optimized *perovskite/Si* tandem SC and its sub-cells are summarized.

Cell type	$V_{oc}(V)$	$J_{sc}(mA/cm^2)$	\boldsymbol{FF} (%)	PCE(96)
Si (Optimal condition)	0.75	34.39	85.47	22.28
$Cs_2AgBiBr_6$ (Optimal condition)	1.01	27.90	86.45	24.44
Top Cell (400 nm)	0.928	24.89	80.50	18.61
Bottom Cell (under filtred spectrum)	0.7493	24.89	85.37	22.77
Perovskite / Si Tandem Cell	1.6773	24.89	86.87	36.26

Results of this study's comparison to real and simulated *perovskite* tandem solar cells.

conducting current matching for various absorber layer values in the top sub-cell, the two sub-cells were also connected to create a suggested tandem device. Tandem solar cells performed best with an absorber bandgap of 1*.*417 *eV* and a thickness of 400 *nm*, resulting in a *PCE* of 36*.*28% and a current density of 24*.*89 *mA/cm*2. We found that the bandgap can be better controlled by employing perovskite in the top cell, which is essential for increasing solar cell efficiency. We believe that by clarifying the effects of perovskite thickness and charge density on cell performance, this study contributes to the body of knowledge on all-perovskite tandem solar cells. Future research and development of highly effective and reasonably priced tandem devices might be guided by the suggested design and optimization strategy.

4. Data accessibility declaration

Data will be provided upon request.

Statement of financial interests

The authors state that they have no conflicts of interest.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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