



STRUCTURAL SIMULATION OF CS₂AGBIBR₆/CS₂AGBIBR₆-BASED PEROVSKITE HETEROJUNCTION SOLAR CELL

Nahid Akhter Jahan^{1,*}, Anik Das^{1,‡}, Md. Humaon Kabir^{1,†}, Md. Asif Hossain^{1,§}

¹Department of Electrical and Electronic Engineering, Southeast University, Bangladesh

Abstract— This article exhibits the performance analysis based on simulative investigation of a non-toxic, lead-free PIN type perovskite heterojunction solar cell (PTSC) with the inclusion of Cs₂AgBiBr₆ as the intrinsic type absorber layer, CsSnI₃ or CsSnBr₃ as the P-type absorber layers, CuSCN as the hole transport layer (HTL), TiO₂ as electron transport layer (ETL), and CdS as Transparent conductive layer (TCO), respectively. From our first proposed structure, we attained an outstanding power conversion efficiency (PCE) of **37.98%** when a CsSnI₃ as P-type absorber at optimum thickness of 300 nm was included. From the second proposed device structure, we achieved highest PCE of **37.77%** when CsSnBr₃ replaced the P-type absorber at the same optimum thickness of 300 nm. The device functioned optimally when the electron affinities were set at 3.2 eV, 4.190 eV, 4.470 eV and 3.4 eV for n-TiO₂, Cs₂AgBiBr₆, CsSnI₃ and CuSCN, respectively. We observed the effect of thickness and doping density on the device's performance of different charge transport layers. Inclusively, this simulation results will render perceptive guidance towards producing an environmentally benign PTSC through pertinent observation of the transport mechanism and understanding of the role of a suitable TCO and an HTM on the routine features of PIN type perovskite heterojunction solar cell.

Keywords— Cs₂AgBiBr₆, CsSnI₃, CsSnBr₃, perovskite heterojunction solar cell (PTSC), ETL, HTL, PCE, TCO.

I. INTRODUCTION

The world is now grappling with the burning need of clean and renewable energy driven power production only for the demand of the elimination of greenhouse gas emission generated from fossil fuel based energy consumption. Among the accessible renewable-energy sources, solar power is considered as the most plenteous

particularly for South Asian countries due to adequate sun irradiance. Hence, we can see that the use of photovoltaic (PV) solar cells is on the progress and certainly, their application will play significant role in future sustainable energy systems.

Although currently in terms of commercial aspect Si-based PVs are the most commonly used cells, however they render a few major limitations such as restricted efficiency and demanding cost [1–6]. Therefore, some other evolving PV technologies [7] such as organic PV, hybrid organic-inorganic PV cells [8,9], dye-sensitized PV cells [10], quantum dots or low-dimensional heterostructure based PVs [11] and perovskite PV cells [12,13] which have appealed the scientists owing to their promising features. Such as, Halide based perovskites (ABX₃) are gaining attention because of suitable light capturing attribute and considered as third generation of PV. They have also created applications as memory devices, LED's, LASER's and detectors [14–16]. In overall, this perovskites exhibit cubic structure with ABX₃ composition, where A = organic monovalent cation (for example CH₃NH₃⁺, CH₃(NH₂)₂⁺), B = metal divalent cation (for instance Pb²⁺, Sn²⁺, or Ge²⁺) and X may belong to Halogen family (X = I, Br, Cl). Recently, organic-inorganic halide perovskites have attained substantial interest as potential candidates in the field of photovoltaics industry due to its favorable optoelectronic properties such as enhanced absorption-coefficient, longer electron and hole diffusion length, suitable charge carrier mobility, recombination lifetime, and less-challenging fabrication procedures [8,9,12,13]. Within less than a decade, the PCE of perovskite PV cells have reached a record more than 25%, exceeding the performance of conventional CdTe/Cu(In, Ga)Se₂-based

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*Corresponding Author: Dr. Nahid Akhter Jahan, Associate Professor, Department of Electrical and Electronic Engineering, Southeast University, 251/A & 252 Tejgaon I/A, Dhaka 1208, Bangladesh. Email: dnaj1983@gmail.com.

‡Anik Das, under-graduate student of 25th batch from the Department of Electrical and Electronic Engineering, Southeast University, 251/A & 252 Tejgaon I/A, Dhaka 1208, Bangladesh. Email: info.anikdas7@gmail.com.

†Md. Humaon Kabir, under-graduate student of 25th batch from the Department of Electrical and Electronic Engineering, Southeast University, 251/A & 252 Tejgaon I/A, Dhaka 1208, Bangladesh. Email: humaonkabir.eee@gmail.com.

§Md. Asif Hossain, Assistant Professor, Department of Electrical and Electronic Engineering, Southeast University, 251/A & 252 Tejgaon I/A, Dhaka 1208, Bangladesh. Email: asif.hossain@seu.edu.bd.



thin-film PV cells [19], whereas, the tandem metal halide perovskites have achieved more than 26% of efficiency, surpassing the crystalline silicon [20–21]. Nevertheless, the organic elements (MA and FA) causes poorer instability under several ambient conditions and thus compromises with the overall performance [22–24]. It is often proven that replacing these organic counterparts by inorganic alkali cations such as Cs⁺ or Rb⁺ can resolve this problem [25,26]. Recently, inorganic CsPbX₃ perovskites are investigated as a budding candidate for efficient PSCs due to better thermal stability. However, although the Pb-based perovskites offers high figure of merits, their viable application is mired due to the moist and heat instability, and together with the toxicity of lead—which cause serious damage in the environment and can cause low and premature birth rates, cancer in circulatory system, brain-cell damage and kidney failure. These urges the researchers to give emphasis on Pb-free, non-toxic alternatives. Recently, substitution of Pb with Sn and Ge is found reliable due to comparable electronic features [27]. Sn seems fairly suitable; particularly acts as favorable candidate for bulk scale production owing to the longer oxidation state, appropriate absorption coefficient (>105 cm⁻¹), finest forbidden-gap (1.2-1.62 eV) and well air stability [28–30]. So far, the maximum efficiency of lead-free perovskite based solar cells is achieved 13.24% for fine-based structure [31]. It was reported that perovskite materials (ABX₃) with Br in the X-site position could render greater stability compared to its I equivalent [32]. With the exchange of I with Br, orthorhombic phase of CsSnI₃ converts into cubic phase of CsSnBr₃, and can render better electronic properties such as increased open circuit voltage in mixed halides [32]. In line with this, halide double perovskite expressed by the form of A₂M'M''X₆ (A is a monovalent cation, M' and M'' are monovalent and trivalent metal ions), has also become favorable alternatives. It also offers high environmental stability, suitable optoelectronic properties, reduced toxicity, and can be considered as good substitute for Pb-based perovskites. For example, lead-free, Bi-based Cs₂AgBiBr₆ halide double perovskite can be a good candidate for PV solar cell. Its thermal and atmospheric stability, lengthy carrier lifetime, better absorption coefficient, and suitable bandgap (ranging from 1.83 eV to 2.19 eV) make it proper as the absorber layer [33]. Too, this perovskite crystallizes in the elpasolite structure, absorbs light in the visible range of the solar radiation [33]. Even though these all-inorganic perovskite based solar cells have shown remarkable growth in the recent years, however, there remains substantial concern in increasing the merits of all-inorganic perovskite solar cells through collective optimization of the absorber layers and its interface.

In this work, we have systematically studied the structural, electronic, and optical properties of two slightly different heterojunction structures with lattice matched HTL and ETL having apposite electron affinities. Besides, the photovoltaic performance of our halide perovskites (Cs₂AgBiBr₆/CsSnI₃ and Cs₂AgBiBr₆/CsSnBr₃) has been observed by varying the thickness and doping concentrations.

II. STRUCTURAL SPECIFICS AND SIMULATION METHOD OF PROJECTED PHOTOVOLTAIC CELLS

In this simulation, we proposed two slightly different devices having the heterojunction architecture of n-type CdS/n-type TiO₂/I-type Cs₂AgBiBr₆/p-type CsSnI₃/p-type CuSCN and n-type CdS/ n-type TiO₂/I-type Cs₂AgBiBr₆/ p-type CsSnBr₃/p-type CuSCN, respectively. We witnessed the effect of absorber thickness, the doping density, absorber defect density, radiative recombination rate (band-to-band), the electron affinity of HTL and ETL, back contact work function, on the overall performance of our device. We are hopeful that these simulation results will contribute to the laboratory based fabrication of non-toxic, and viable halide based PTSC.

A. Selection of HTL, ETL and absorbers for the devices

The inclusion of electron/hole-transport materials (ETL/HTL) in the PTSC is very crucial for extracting photo-generated excitons from the perovskite absorber layer to the outer contacts. Selection of ETL and HTL is vital for active carrier transport at the interface mostly due to the energy band arrangement; the ETL pulls electrons while obstructing the holes and HTL pulls holes by obstructing holes. The mostly met ETL materials in PVSCs are Fe₂O₃, SnO₂, ZnO, TiO₂, In₂O₃, a-IGZO and PCBM [34–36]. Among these, TiO₂ is found as the most usually and oftenly used ETL owing to its some attractive attributes such as low-cost, high electron mobility, low-ecotoxicity and stability.

The utmost common material for HTL are Spiro-OMeTAD, PEDOT:PSS, P3HT, and PTAA. However, due to their costly fabrication procedure and low chemical durability many researches have been trying to find some other auxiliary. In addition, some inorganic HTL (Cu-based) such as CuSCN, CuI, Cu₂O, and CuO_x are proposed as relevant materials owing to their quicker hole mobility, chemical durability and moderate-fabrication-cost [37,38].

Likewise, insertion of effective absorber layers in tandem cells and their proper alignment of energy bands with transport layers [10] is one of the prime concerns for effective passage or collection of the charge carriers to the metallic-contacts. This is basically possible if the work-

function of front contact material is nearly matching or marginally larger than conduction band edge of the transport layer. Consequently, higher work-function presumably yields an ohmic contact for holes and electrostatic barrier for electrons in HTL. Cell performance also deteriorates if the recombination mechanism is not addressed properly as gathered charges will influence the electric field inside the cell. Thus appropriate buffer layer is vital to maintain the current flow through an entire tandem architecture. In light of the above issues, we have identified $\text{Cs}_2\text{AgBiBr}_6$ as an thin intrinsic (I) layer and act as low dimensional quantum confined absorber layer that can capture more excitons in the vicinity of wide p-type absorbers (CsSnI_3 or CsSnBr_3). This $\text{Cs}_2\text{AgBiBr}_6$ is all-inorganic, lead-free perovskite, which adopt the ideal cubic structure with very close lattice parameters and particularly lattice matched with CgSnBr_3 at room temperature. Such combination minimizes interference defect states from complex compositions of crystal structures.

B. Simulation method for the devices

The well-known SCAPS-1D simulation program/software (version 3307) is used in this study to carry out the modeling and simulation. SCAPS-1D is a one-dimensional simulator facilitating maximum seven semiconductor layers and it tasks based on Poisson and Continuity equations to model and simulate numerous PV structures. This simulator can calculates energy bands, concentrations and currents, J-V characteristics, spectral response (QE). This solar cell simulator has been widely used for the device modeling of solar cells and results almost validate the experimental results. The calculation was done under 1.5 AM solar irradiance and at a temperature of 300 K.

The all requisite design parameters used for the device modelling of the structures are given in Table-I and II; collected from formerly reported literatures [33,39].

In Figure 1 (a), the structural details of our proposed PIN type two different structures are shown pictorially. In our first proposed structure, CdS is inserted as n-type (optimized 10 nm thick) at the top, TiO_2 is used as n-type (optimized 20 nm thick) ETL, $\text{Cs}_2\text{AgBiBr}_6$ is utilized as an intrinsic type absorber (optimized 10 nm) and the p-type CsSnI_3 (300 nm thick) is sandwiched as the absorber layer. Thereafter a p-type CuSCN (optimized at 20 nm) is inserted as HTL. The total thickness of the entire structure becomes only 360 nm as a whole. From the point of view of fabrication suitability due to favorable lattice matching, we studies another structure that is almost similar; only the p-type CsSnI_3 is replaced by the p-type CsSnBr_3 shown in Figure 1 (b).

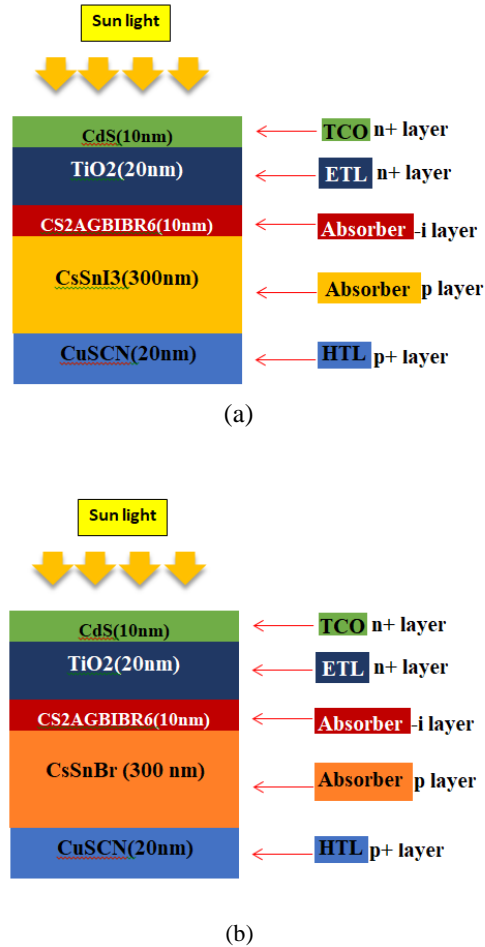


Fig. 1. (a) Schematic depiction of the first proposed structure [lead-free PIN type perovskite heterojunction solar cell (PTSC) with the inclusion of $\text{Cs}_2\text{AgBiBr}_6$ as the intrinsic type absorber layer, CsSnI_3 as the P-type absorber layers, CuSCN as the hole transport layer (HTL), TiO_2 as electron transport layer (ETL), and CdS as Transparent conductive layer (TCO)].

(b) Schematic representation of the second PTSC with the inclusion of $\text{Cs}_2\text{AgBiBr}_6$ as the intrinsic type absorber layer, CsSnBr_3 as the P-type absorber layers, CuSCN as the hole transport layer (HTL), TiO_2 as electron transport layer (ETL), and CdS as Transparent conductive layer (TCO)

TABLE I
 PARAMETERS OF KEY MATERIALS UTILIZED AS ABSORBER LAYER

Parameter	$\text{Cs}_2\text{AgBiBr}_6$	CsSnI_3	CsSnBr_3
Thickness (nm)	10 nm	300 nm	300 nm
E_g (eV)	2.05	1.270	1.110
χ (eV)	4.190	4.470	4.460
ϵ_r	5.800	10.590	6.400
N_c (cm^{-3})	1.00×10^{20}	1.8×10^{19}	1.5×10^{19}



$N_v(cm^{-3})$	1.800×10^{19}	1.67×10^{18}	1.47×10^{18}
$V_{e-th}(cm/s)$	1×10^7	1×10^7	1×10^7
$V_{p-th}(cm/s)$	1×10^7	1×10^7	1×10^7
$\mu_c(cm^2/V_s)$	1.181×10^1	3.11×10^2	4.37×10^2
$\mu_p(cm^2/V_s)$	4.90×10^{-1}	4.2×10^1	4.37×10^1
$N_D(cm^{-3})$	1×10^{19}	0	0
$N_A(cm^{-3})$	1×10^{19}	5×10^{19}	5×10^{19}

TABLE II
PARAMETERS OF MATERIALS USED AS ETM, TCO AND HTM

Parameter	n-TiO ₂	n-CdS	p-CuSCN
Thickness (nm)	20 nm	10 nm	20 nm
$E_g(eV)$	3.2	2.4	3.4
$\chi(eV)$	4.2	4.2	2.1
ϵ_r	9	9	10
$N_c(cm^{-3})$	2.2×10^{18}	2.2×10^{19}	2.5×10^{18}
$N_v(cm^{-3})$	1.8×10^{19}	1.8×10^{18}	1.8×10^{19}
$V_{e-th}(cm/s)$	1×10^7	1×10^7	1×10^7
$V_{p-th}(cm/s)$	1×10^7	1×10^7	1×10^7
$\mu_c(cm^2/V_s)$	2×10^1	1×10^2	2×10^{-4}
$\mu_p(cm^2/V_s)$	1×10^1	2.5×10^1	1×10^{-2}
$N_D(cm^{-3})$	1×10^{18}	3.0×10^{18}	0
$N_A(cm^{-3})$	0	1×10^1	1×10^{18}

III. RESULTS AND DISCUSSIONS

An effective heterojunction cell demands a few conditions, such as: the short circuit throughout the multi-junctions should be properly matched and the PV will offer smallest, generation of excitons against wide range of solar irradiance should be effective while the electrical resistance and optical losses should be as low possible.

These necessities can be controlled by varying band-gap, thickness, and by including suitable transport layer with suitable affinity levels.

It has been known that the PV cells typically gives higher efficiency if light enters into the cell from P-type window. As our structure is a PIN type we have chosen p-type-CsSnX₃ (X= I or Br) as the prime absorber layer which absorbs mostly the photons of visible to near infrared wavelength. The intrinsic (I) layer works as additional absorber layer that can capture multiple photons of higher energies due to its confined energy states attributed to 10 nm thickness and will also offer high electric field due to small thickness. On the other hand, wider p-type-CsSnX₃ will soak more carriers due its wider thickness. Then the generated carriers experience the field, swept towards the outer contact of the structure pulled by the ETL/HTL. As a result, it is projected that the thickness, energy gap, and defect states of the I-layer are crucial design characteristics.

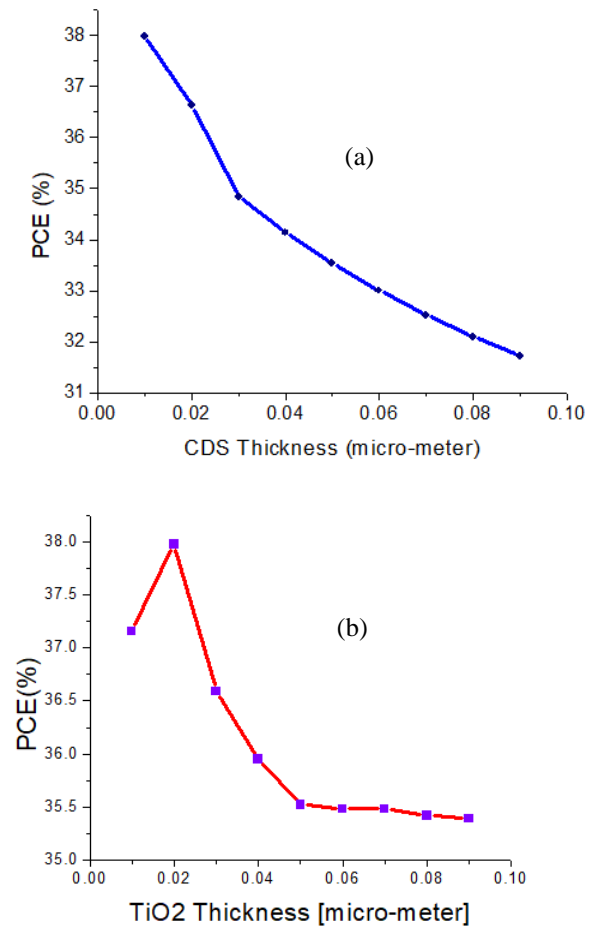


Fig. 1. The PCE as a function of varying thickness from 10 nm to 90 nm for (a) TCO (CdS) and (b) ETL (TiO₂).

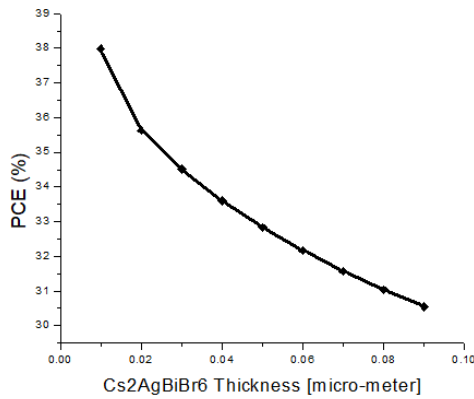


Fig. 2. The PCE as a function of thickness from 10 nm to 90 nm for Cs₂AgBiBr₆ as I type absorber layer.

Our simulation, as shown in Figure 1, shows the effect of varying thickness on the performance of the cell; exemplarily the power conversion efficiency (PCE) is depicted. We can see that the optimized thickness of TiO₂ is achieved as 20 nm and for CdS the suitable thickness is found as 10 nm. The maximum PCE is achieved 39.88% with FF of 83.12%, open circuit voltage V_{oc} of 1.17 V and short circuit current J_{sc} of 39.19 mA/cm². Table III and IV depicts the obtained simulation result for ETL (TiO₂) and TCO (CdS).

Table III

Performance optimization of PTSC for ETL, TiO ₂				
Thickness	V _{oc} (Voltage)	J _{sc} (mA/cm ²)	FF (%)	PCE%
0.01	1.17	38.27	83.11	37.16
0.02	1.17	39.19	83.12	37.98
0.03	1.17	37.25	81.98	36.59
0.04	1.17	37.2	81.99	35.55
0.05	1.17	37.16	81.99	35.52
0.06	1.17	37.13	82	35.48
0.07	1.17	37.09	82.01	35.48
0.08	1.165	37.06	82.01	35.42
0.09	1.165	37.02	82.02	35.39

Table IV

Performance optimization of PTSC for TCO, CdS				
Thickness	V _{oc} (Voltage)	J _{sc} (mA/cm ²)	FF (%)	PCE%
0.01	1.17	39.19	83.12	37.98
0.02	1.17	38.27	82.22	36.63
0.03	1.17	36.47	81.99	34.84
0.04	1.16	35.77	81.97	34.15
0.05	1.16	35.15	81.95	33.54
0.06	1.16	34.61	81.93	33
0.07	1.16	34.12	81.91	32.52
0.08	1.16	33.69	81.9	32.09
0.09	1.16	33.31	81.88	31.72

Similarly, we can see from the Figure 2 that the maximum PCE is obtained at 10 nm thickness for Cs₂AgBiBr₆ absorber layer (Table V shows the details).

Table V

Performance optimization of PTSC for Cs ₂ AgBiBr ₆				
Thickness	V _{oc} (Voltage)	J _{sc} (mA/cm ²)	FF (%)	PCE%
0.01	1.17	38.27	83.11	37.98
0.02	1.17	37.27	82.02	35.63
0.03	1.17	36.55	80.97	34.51
0.04	1.17	36.02	79.99	33.6
0.05	1.17	35.6	79.05	32.84
0.06	1.17	35.26	78.16	32.17
0.07	1.17	34.96	77.32	31.57
0.08	1.17	34.71	76.53	31.04
0.09	1.17	34.48	75.79	30.55

On the contrary, we see from the Figure 3 that the PCE remains almost constant until 70 nm of thickness for HTL (CuSCN). We chose a thickness of 20 nm from the viewpoint of cost optimization.

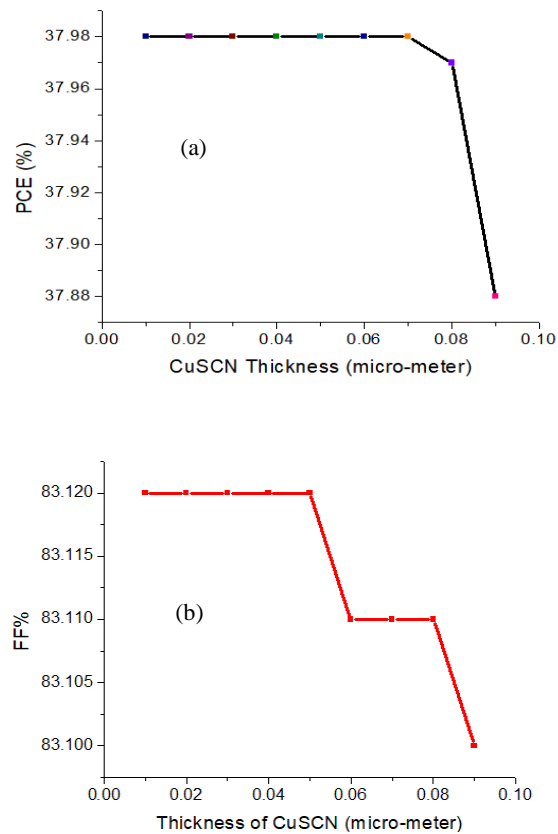


Fig. 3. The effect of the variation of thickness on (a) PCE and (b) FF of the entire structure for the HTL (CuSCN).

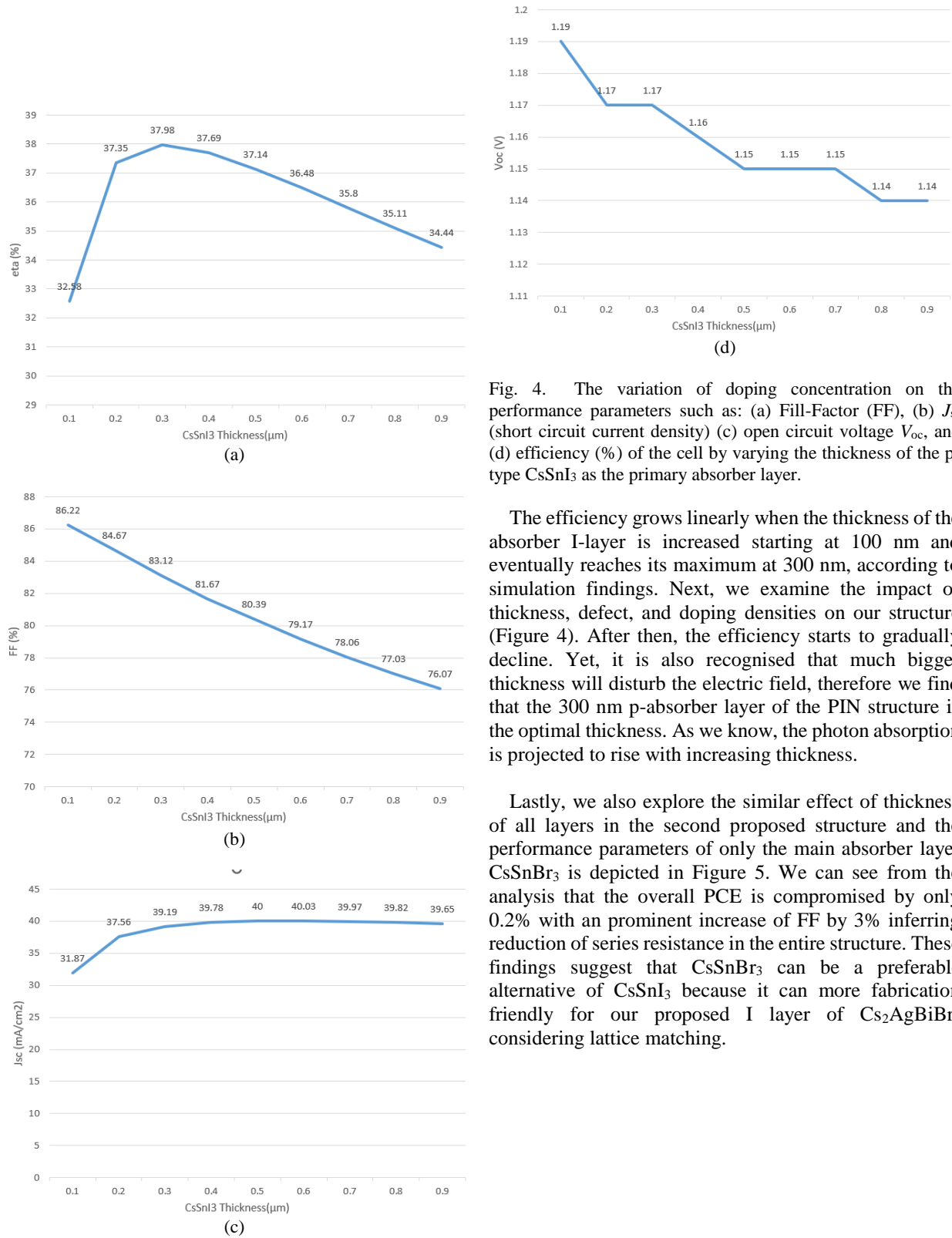


Fig. 4. The variation of doping concentration on the performance parameters such as: (a) Fill-Factor (FF), (b) J_{sc} (short circuit current density) (c) open circuit voltage V_{oc} , and (d) efficiency (%) of the cell by varying the thickness of the p-type CsSnI₃ as the primary absorber layer.

The efficiency grows linearly when the thickness of the absorber I-layer is increased starting at 100 nm and eventually reaches its maximum at 300 nm, according to simulation findings. Next, we examine the impact of thickness, defect, and doping densities on our structure (Figure 4). After then, the efficiency starts to gradually decline. Yet, it is also recognised that much bigger thickness will disturb the electric field, therefore we find that the 300 nm p-absorber layer of the PIN structure is the optimal thickness. As we know, the photon absorption is projected to rise with increasing thickness.

Lastly, we also explore the similar effect of thickness of all layers in the second proposed structure and the performance parameters of only the main absorber layer CsSnBr₃ is depicted in Figure 5. We can see from the analysis that the overall PCE is compromised by only 0.2% with an prominent increase of FF by 3% inferring reduction of series resistance in the entire structure. These findings suggest that CsSnBr₃ can be a preferable alternative of CsSnI₃ because it can more fabrication friendly for our proposed I layer of Cs₂AgBiBr₆ considering lattice matching.

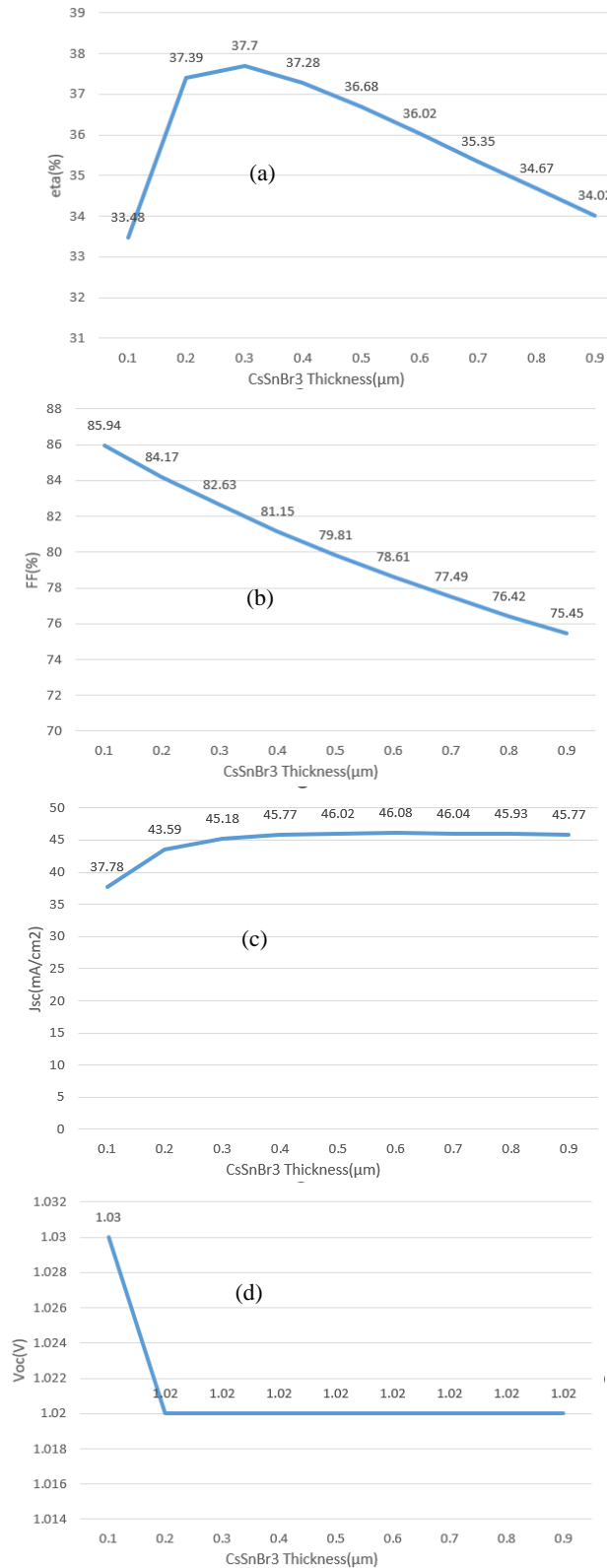


Fig. 5. The variation of doping concentration on the performance parameters (a) Fill-Factor (FF), (b) J_{sc} (short circuit current density) (c) open circuit voltage V_{oc} , (d) and efficiency

(%)) of the cell by varying the thickness of the p-type $CsSnBr_3$ as the absorber layer.

Lastly, the screenshot of the I-V curve from SCAPS-1D following the simulation of the second proposed PTSC, the calculated energy diagram, the calculated recombination current densities and the internal quantum efficiency curve are shown in Figure 6, Figure 7 and the plotted I-V curve of the same structure is shown in Figure 8, respectively for the readers understanding.

A Table VI compares the key performance merits of $Cs_2AgBiBr_6/CsSnI_3$ and $Cs_2AgBiBr_6/CsSnBr_3$ based device acquired in this work, as well as with those reported previously. We can see that our structure offers outstanding performance with the inclusion of lead free absorbers in both PTSCs. We hope this will motivate the researchers who are interested in perovskite based new generation of solar cell design.

TABLE VI
 COMPARISON WITH PREVIOUS WORK

Device	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
$CdS/TiO_2/Cs_2AgBiBr_6/CsSnI_3/CuSCN$ (our proposed device 1)	1.17	39.19	83.12	37.98
$CdS/TiO_2/Cs_2AgBiBr_6/CsSnBr_3/CuSCN$ (our proposed device 2)	1.03	37.78	85.94	37.77
$ZnO-NR/Cs_2AgBiBr_6/P3HT$ (Base) [33]	0.92	11.10	44.02	4.48
$FTO/ZnO/Cs_2AgBiBr_6/NiO/Au$ [40]	1.29 V	20.69	81.72	21.88

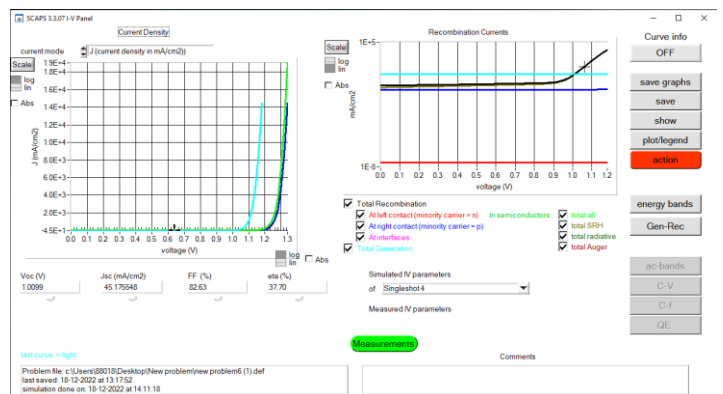


Fig. 6. The screen-shot image of the I-V curve from SCAPS-1D after simulation of the second proposed PTSC

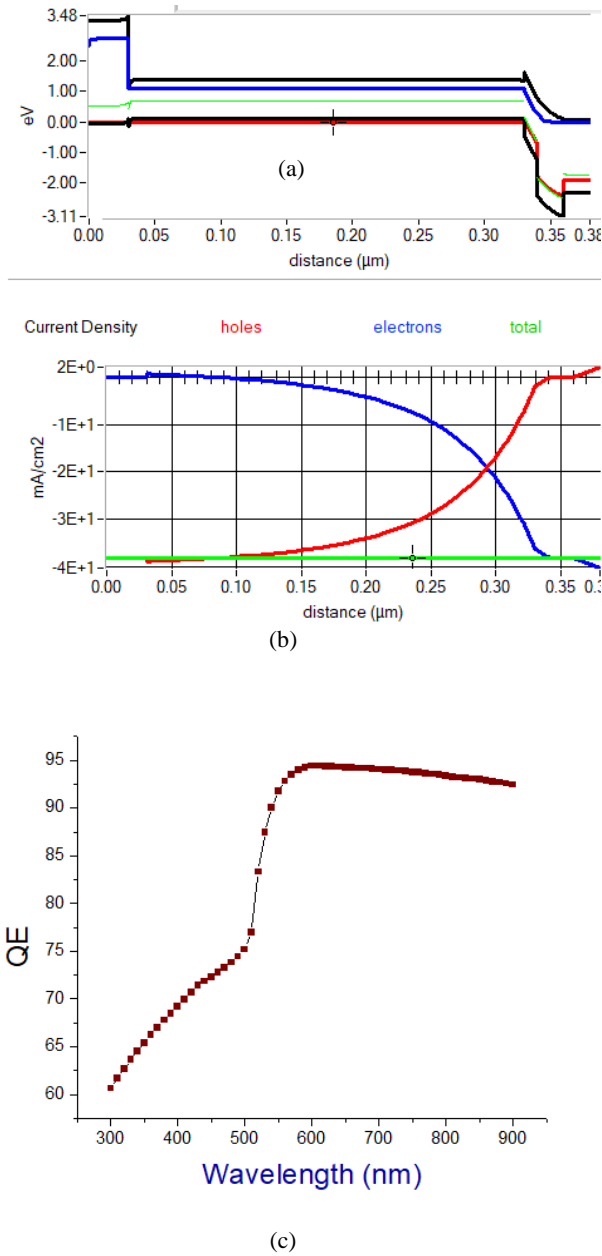


Fig. 7. (a) The calculated energy diagram. (b) The calculated recombination current densities and (c) The quantum efficiency curve.

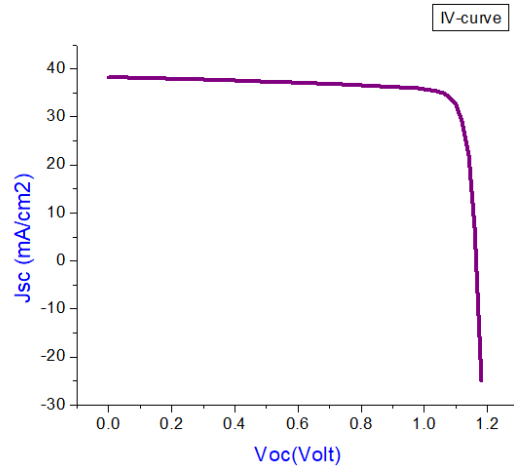


Fig. 8. The I-V characteristics of the PIN type PTSC for $Cs_2AgBiBr_6/CsSnBr_3$.

IV. CONCLUSION

In this paper, a methodical analysis two types of tandem PIN devices $n-CdS/n-TiO_2/I-Cs_2AgBiBr_6/p-CsSnI_3/p-CuSCN$ and $n-CdS/n-TiO_2/I-Cs_2AgBiBr_6/p-CsSnBr_3/p-CuSCN$, PV cells are modelled and calculated using SCAPS-1D simulator. The devices were simulated and optimized to gain best figure of merits by varying thickness, defect densities and doping densities of all layers. The highest PCE is achieved as 37.88% implementing $Cs_2AgBiBr_6$ as thin I-type absorber layer with $CsSbI_3$ as suitable wide P-type exciton generation layer. The another structure results in almost same PCE of 37.77% by replacing the $CsSbI_3$ with $CsSbBr_3$. Since $Cs_2AgBiBr_6$ is an ideal, cubic structure with very close lattice matched with $CsSnBr_3$ at room temperature. This combination of $Cs_2AgBiBr_6$ with $CsSnBr_3$ certainly minimizes interference defect states from complex compositions of crystal structures. The findings of the simulation show that they played a key role in reaching such a high efficiency.

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Dr. Nahid A Jahan was born in 20th April 1983 in Rajshahi. She received her B. Sc. (2005) and M. Sc. (2007) in Applied Physics & Electronic Engineering (APEE), Rajshahi University, Bangladesh. She did her PhD (2013) in the field of Electronics for Informatics from Laboratory of Nanophotonics, Research Institute for Electronic Science (RIES) under graduate school of Information Science and Technology, Hokkaido University, Japan. Thereafter she got post-doctoral research fellowship in the same Laboratory of Nanophotonics, Research Institute for Electronic Science (RIES), Hokkaido University, Japan. Currently, she is working as an Associate Professor in the Department of Electrical and Electronic Engineering (EEE) of Southeast University, Dhaka, Bangladesh. Previously, she worked at the East West University of Bangladesh, Dhaka as an Associate Professor in the department of ECE (until 2018). So far, she has published over 16 research papers in national and international journals and presented 18 papers in international conferences. She is the member of IEEE, and JSAP. She is a regular reviewer and organizing committee member of several national and international journals and conferences. The whole gamut of her research interests and activities encompass multidisciplinary domains/fields. During the course of her PhD and postdoctoral studies, she carried out research on nanophotonics semiconductor nanostructures, quantum optics, cavity quantum electrodynamics, quantum information science and engineering. Alongside, she pursued research on developing an apposite plasma assisted synthesis method for the production of nano/micro materials. It is worth mentioning that seeing the ubiquitous demand of energy supply, its constraints, and the repercussion on environment, throughout her teaching career/experience in the Universities of Bangladesh she has been entirely working for Sustainable Clean Energy /Renewable Energy, Multijunction Photovoltaic Cell Design, Electric Vehicles and its impacts on the Environment and Power Grid.



Anik Das was born in Dhaka, Bangladesh. He has been studying in the Department of Electrical and Electronic Engineering, Southeast University, Bangladesh. His

present research interests involve the following focuses: Design and Simulation of High efficiency Multi junction Thin Film Solar Cells. Design and Simulation of Highly efficient and non-toxic Perovskite based Solar Cells.



Md. Humaon Kabir was born in Dhaka, Bangladesh. He has been studying in the Department of Electrical and Electronic Engineering, Southeast University, Bangladesh. His present research interests involve the following focuses: Design and Simulation of Semiconductor Device. Design and Simulation of non-toxic Perovskite based Solar Cells.



Dr. Md. Asif Hossain received his B.Sc. degree in Information and Communications Engineering, M.Sc. degree in Telecommunications Engineering, and MBA degree in Marketing from East West University (EWU), Dhaka, Bangladesh, in 2006, 2007, and 2011, respectively. He was a recipient of Chancellor's Gold Medals for his excellent performance in his B.Sc. and M.Sc. degrees. He achieved his Ph.D. degree in Computer Science at the University of Malaya in Malaysia. Currently, he is working as an Assistant Professor in the Department of Electrical and Electronic Engineering (EEE) at Southeast University, Dhaka, Bangladesh. Previously, he worked as an Assistant Professor at the Department of Electronics and Communications Engineering at East West University, Dhaka, Bangladesh. His research interests include cognitive radio, vehicular networks, wireless networking, machine learning, energy harvesting and SWIPT. So far, he has published 33 articles that include 19 peer-reviewed international journal papers, a book chapter, 9 international conference proceedings with best paper and presentation awards, and 4 national conference proceedings. He is a recipient of several international grants.