



# Device Engineering of Lead-free Double Perovskite ( $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$ & $\text{Cs}_2\text{AgBiBr}_6$ )/Crystalline Silicon High-Performance Eco-friendly Tandem Solar Cells

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Received: 27 November 2023 / Accepted: 15 February 2024 / Published online: 2 March 2024  
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## Abstract

Lead-free double perovskites are a newly developed category of non-toxic material with impressive photoelectric properties and excellent inherent environmental stability. This study explores the design and performance optimization of lead-free double perovskite/c-Si tandem devices (TDs). Two top cells (TCs) made of  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  (bandgap of 1.6 eV) and  $\text{Cs}_2\text{AgBiBr}_6$  (bandgap of 2.05 eV) absorber materials and the bottom cell (BC) of c-Si (bandgap of 1.12 eV), have been utilized for designing two TDs. To design an efficient TD's structure, TC and BC were first individually simulated and calibrated against the findings derived from the reported experimental data. The absorber's thickness of TC reaches the current matching, when the current it generates under AM 1.5G spectrum matches the BC's current under a filtered spectrum (generated through TC). At current matching condition, the optimized values of thickness of  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  and  $\text{Cs}_2\text{AgBiBr}_6$  layers are 0.418 and 1.29  $\mu\text{m}$ , respectively. The lead-free  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}/\text{c-Si}$  and  $\text{Cs}_2\text{AgBiBr}_6/\text{c-Si}$  TDs exhibit a PCE (power conversion efficiency) value of 34.67% ( $V_{\text{OC}} = 1.82$  V,  $J_{\text{SC}} = 20.75$  mA/cm<sup>2</sup>, FF = 88.31%) and 36.88% ( $V_{\text{OC}} = 2.16$  V,  $J_{\text{SC}} = 21.105$  mA/cm<sup>2</sup>, FF = 79.68%), respectively. Performance parameters of TDs obtained from this work are comparable to the results of reported experiments and simulations. Analysis of this study reveals that enhancing PCE of double-perovskite TC is essential to promise the TD's benefits. The results reported demonstrate that lead-free and stable double perovskite materials can act as an essential absorber in sub-cells for highly efficient, commercially viable, non-toxic and eco-friendly tandem photovoltaic technologies.

**Keywords** Current matching ·  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  ·  $\text{Cs}_2\text{AgBiBr}_6$  · Lead-free double perovskite · Power conversion efficiency (PCE) · Tandem solar device

## 1 Introduction

The need to develop more efficient, cost-effective, and eco-friendly renewable energy sources is growing as a result of the rising energy demand, which has led to major environmental concerns. Photovoltaic (PV) technology is widely recognized as one of the cleanest and most sustainable energy options available. It enables the direct transformation of solar energy into electricity. Silicon (Si)-PV, presently dominating the PV industry, has achieved an efficiency

milestone of 26.7% [1, 2], approaching the 33% limit (Shockley-Queisser limit) for single-junction PV/ solar cells [3, 4]. To address this limitation, the combination of multiple single-junction PV cells, each having distinct bandgaps, to form a multi-junction or tandem device (TD), enables a broader absorption of photons from the solar spectrum while minimizing energy loss [5, 6]. Under AM 1.5G illumination, it is theoretically possible for an infinite stack of junctions to attain a power conversion efficiency (PCE) of 65.4%. This suggests the potential for highly efficient energy conversion in multi-junction solar cell configurations [7]. Tandem solar cells (TSCs) exist in many design configurations based on their electrical connections and manufacturing processes. The electrical series connection of top cell (TC) and bottom cell (BC) in TSCs ensures that current passing through both cells remains constant [8, 9]. Several tandem solar device configurations are still being thoroughly explored.

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Perovskite solar cells (PSCs) present favourable choices for integration into TDs owing to their outstanding absorption, bandgap tuning capabilities, and affordable deposition methods [10, 11]. Perovskite has successfully been used in demonstrations of high-efficiency Si-based TDs. The investigation of Perovskite/Si TDs to improve PCE has been promising [12]. Perovskite/Si TDs (both monolithic, as well as mechanically stacked) are commercially feasible technologies in recent times, showing PCE of more than 30% [13]. Recent breakthroughs in organic-inorganic halide PSCs have resulted in a significant increase in PCE, escalating from a mere 3% in 2006 to an impressive 25.8% at present [14–17]. Despite their rapid efficiency improvements, PSCs face persistent challenges that hinder their transition into a competitive market viability [18–20]. The primary concerns revolve around the toxicity and stability issues associated with lead-based PSCs, posing obstacles to their widespread commercialization [21]. In addressing these concerns, tin (Sn), which shares a comparable atomic size, has been considered as a substitute for lead (Pb), forming  $\text{ASnX}_3$  structures in lead-free lead-free PSCs. Sn-based PSCs often exhibit lower efficiencies than lead-based counterparts, due to the inherent instability of  $\text{Sn}^{2+}$  ions, prone to oxidation and transformation into  $\text{Sn}^{4+}$ . This oxidation adversely affects material stability, posing a significant challenge in improving performance [21, 22]. Developing novel stable and lead-free perovskites for PV applications remains challenging. Introducing a double perovskite structure offers a potential avenue for expanding perovskite applications in photovoltaics. This entails replacing two  $\text{Pb}^{2+}$  ions with one  $\text{M}^+$  and one  $\text{M}^{3+}$  ions, resulting in an  $\text{A}_2\text{M}^+\text{M}^{3+}\text{X}_6$  double perovskite structure [23]. Experiments have demonstrated  $\text{Cs}_2\text{AgBiBr}_6$  and  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  are the most typical stable and lead-free double perovskites [24–26]. The reported theoretical optimized PCE of a  $\text{Cs}_2\text{AgBiBr}_6$  and  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  based solar cells are up to 11.69% [24] and 30% [26], respectively. A lead-free and stable tandem solar device with enhanced performance has to be developed.

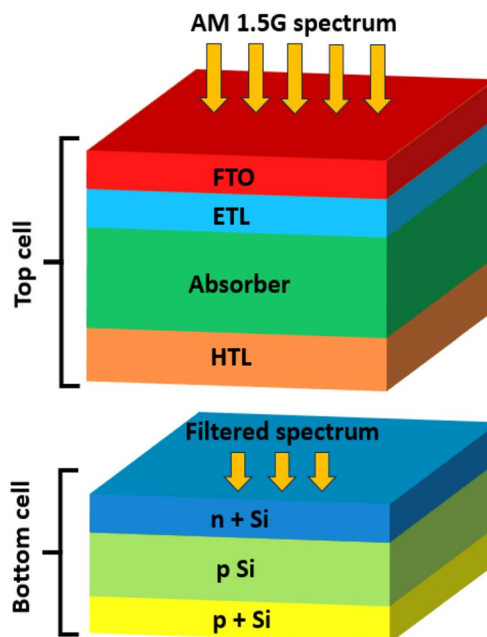
Two lead-free double perovskite/c-Si (crystalline Si) TSCs utilizing  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  and  $\text{Cs}_2\text{AgBiBr}_6$  as the TC's absorber layers have been designed and investigated in this work. In tandem configuration, TC comprises a Hole Transport Layer (HTL), a double perovskite film serving as the absorber, and an Electron Transport Layer (ETL). Both TC (ETL/Absorber/HTL) and BC (c-Si: n+ / p / p+) have been connected in series configuration to construct a two-terminal (2-T) TD. Numerical designs of the devices were conducted using SCAPS-1D (Solar Cell Capacitance Simulator), initially simulating standalone models for both TC and BC, subsequently calibrating them with reported experimental data from existing literature. Furthermore, investigations were undertaken to optimize results by tuning parameters related to the TC's absorber layer and interfaces.

The thickness of the TC's absorber layer is tuned to ensure current matching between the cells. By ensuring current matching conditions, the performance of TD models can be analyzed through device designs of both TC and BC models under the AM 1.5G solar spectrum, and the filtered spectrum, respectively. These designs provide valuable insights into the overall performance of the device, playing a key role in advancing TSC technology. The efficacy of the designed TD models has been validated by comparing their performance with experimental, as well as simulated results reported in existing literature.

In Section 2, the device structure is outlined, elucidating essential input/model parameters for each individual layer. Section 3 delves into the calibration of the sub-cells and outlines the numerical methodology for designing the TDs. Further, the obtained results for lead-free double perovskite/c-Si TDs are presented and discussed in Section 4, followed by a comparison with the recently reported results in Section 5.

## 2 Device Structure and Model Parameters

The schematic diagram for lead-free double perovskite/c-Si (crystalline silicon) TD is represented in Fig. 1. In the proposed TD, the BC is in fact a c-Si solar cell, while the TC is a lead-free double perovskite-based solar cell. Both sub-cells are joined together in a series configuration to form a 2-T TD. Illumination with the AM 1.5G solar spectrum is directed towards TC, whereas BC is subjected to a filtered



**Fig. 1** Schematic representation for lead-free double perovskite/c-Si TD

**Table 1** Device structures for proposed TC, BC and TD models

Cell	Device structure	ID
BC	n + Si/pSi/p + Si	c-Si
TC (ETL/ Absorber/HTL)	TiO <sub>2</sub> /Cs <sub>4</sub> CuSb <sub>2</sub> Cl <sub>12</sub> /Cu <sub>2</sub> O Zn <sub>0.75</sub> Mg <sub>0.25</sub> O/Cs <sub>2</sub> AgBiBr <sub>6</sub> /Cu : Ni <sub>1-x</sub> O	TC-1 TC-2
TD (TC/BC)	TC-1/c-Si TC-2/c-Si	TD-1 TD-2

spectrum generated from the TC. The structure of TC includes a front contact incorporating FTO (Fluorine-doped tin oxide), ETL, lead-free double perovskite film (absorber layer), HTL, and a metallic back contact (Au). For designing of TD, the selected materials for different layers of TC are: TiO<sub>2</sub> and Zn<sub>0.75</sub>Mg<sub>0.25</sub>O as ETL, lead-free double perovskites Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub> and Cs<sub>2</sub>AgBiBr<sub>6</sub> as absorber layer, and Cu<sub>2</sub>O and Cu: Ni<sub>1-x</sub>O as HTL. Having good photoelectric

properties and innate stability, double perovskites are a novel kind of material [24–26]. BC has a base layer that is moderately doped p-type, an emitter that is highly doped p-type, and an n+ (highly doped n-type) layer that serves as BSF (back surface field).

The device structures of the proposed TC, BC and TD models are represented in Table 1. The bandgaps of absorber layers of TC-1 (Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub> as absorber) and TC-2 (Cs<sub>2</sub>AgBiBr<sub>6</sub> as absorber) are 1.6 and 2.05 eV, respectively. All layers of BC have a band gap of 1.12 eV. This study uses SCAPS software, and Tables 2, 3 and 4 list the basic input/model parameters of different layers in sub-cells and interfaces after being carefully chosen from published literature and experimental works [24, 26–31]. All layers, along with interfaces like absorber/HTL and ETL/absorber, are subjected to neutral defects characterized by a single energetic distribution. Figure 2a and b depict energy band diagrams (EBDs) of the diverse materials utilized in sub-cell’s design, offering insights into their respective

**Table 2** Input parameters for different layers of TCs

TC Parameters	TC-1				TC-2			
	FTO	TiO <sub>2</sub>	Cs <sub>4</sub> CuSb <sub>2</sub> Cl <sub>12</sub>	Cu <sub>2</sub> O	FTO	Zn <sub>0.75</sub> Mg <sub>0.25</sub> O	Cs <sub>2</sub> AgBiBr <sub>6</sub>	Cu : Ni <sub>1-x</sub> O
Thickness (nm)	500	30	200 (varied)	200	30	30	200 (varied)	98
Bandgap (eV)	3.2	3.2	1.6	2.17	3.5	3.82	2.05	3.89
Electron affinity (eV)	4.4	4	3.74	3	4	4.03	4.19	1.56
Permittivity	9	9	10	7.5	9	9	5.8	11.7
Effective CB density (cm <sup>-3</sup> )	2.2 × 10 <sup>18</sup>	1 × 10 <sup>21</sup>	4.5 × 10 <sup>19</sup>	2.0 × 10 <sup>18</sup>	2.2 × 10 <sup>18</sup>	1 × 10 <sup>15</sup>	1 × 10 <sup>16</sup>	3.78 × 10 <sup>16</sup>
Effective VB density (cm <sup>-3</sup> )	1.8 × 10 <sup>19</sup>	2 × 10 <sup>20</sup>	1.6 × 10 <sup>19</sup>	1.1 × 10 <sup>19</sup>	1.8 × 10 <sup>19</sup>	1 × 10 <sup>16</sup>	1 × 10 <sup>16</sup>	3.78 × 10 <sup>16</sup>
Electron velocity (cm/s)	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>
Hole velocity (cm/s)	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>	1.0 × 10 <sup>7</sup>
Electron mobility (cm <sup>2</sup> /Vs)	20	0.006	2.5	200	20	50	11.81	5.58
Hole mobility (cm <sup>2</sup> /Vs)	10	0.006	2.5	80	10	20	0.49	5.58
Donor density (cm <sup>-3</sup> )	1.0 × 10 <sup>19</sup>	5.06 × 10 <sup>19</sup>	-	-	1.0 × 10 <sup>18</sup>	1.0 × 10 <sup>16</sup>	1.0 × 10 <sup>19</sup>	-
Acceptor density (cm <sup>-3</sup> )	-	-	1.0 × 10 <sup>13</sup>	2.0 × 10 <sup>19</sup>	-	-	1.0 × 10 <sup>19</sup>	3.0 × 10 <sup>18</sup>
Defect density (cm <sup>-3</sup> )	1.0 × 10 <sup>14</sup>	1.0 × 10 <sup>15</sup>	1.0 × 10 <sup>13</sup>	1.0 × 10 <sup>15</sup>	1.0 × 10 <sup>15</sup>	1.0 × 10 <sup>15</sup>	1.0 × 10 <sup>15</sup>	1.0 × 10 <sup>14</sup>
Extinction coefficient (k)	0.117	0.116	0.304	0.226	0.083	0.027	0.239	0.005
Refractive index (n)	3.002	3.002	3.176	2.747	3.001	3.0	2.42	3.42

**Table 3** Input settings for TC’s absorber/HTL and ETL/absorber interfaces

TC Parameters	TC-1		TC-2	
	Cs <sub>4</sub> CuSb <sub>2</sub> Cl <sub>12</sub> /Cu <sub>2</sub> O	TiO <sub>2</sub> /Cs <sub>4</sub> CuSb <sub>2</sub> Cl <sub>12</sub>	Cs <sub>2</sub> AgBiBr <sub>6</sub> /Cu : Ni <sub>1-x</sub> O	Zn <sub>0.75</sub> Mg <sub>0.25</sub> O/Cs <sub>2</sub> AgBiBr <sub>6</sub>
Defect type	Neutral	Neutral	Neutral	Neutral
Capture cross section for electrons (cm <sup>2</sup> )	3.22 × 10 <sup>-18</sup>	3.22 × 10 <sup>-18</sup>	3.22 × 10 <sup>-18</sup>	3.22 × 10 <sup>-18</sup>
Capture cross section for holes (cm <sup>2</sup> )	3.22 × 10 <sup>-18</sup>	3.22 × 10 <sup>-18</sup>	3.22 × 10 <sup>-18</sup>	3.22 × 10 <sup>-18</sup>
Energetic distribution	Single	Single	Single	Single
Energy with respect to reference (eV)	1.3	1.3	1.3	1.3
Total density (cm <sup>-2</sup> )	2.3 × 10 <sup>10</sup>	2.3 × 10 <sup>10</sup>	2.3 × 10 <sup>10</sup>	2.3 × 10 <sup>10</sup>

**Table 4** Input parameters of different layers of BC

Parameters	n + Si	p Si	p + Si
Thickness ( $\mu\text{m}$ )	0.2	0.3	0.1
Bandgap (eV)	1.12	1.12	1.12
Electron affinity (eV)	4.05	4.05	4.05
Permittivity	11.9	11.9	11.9
Effective CB density ( $\text{cm}^{-3}$ )	$2.8 \times 10^{19}$	$2.8 \times 10^{19}$	$2.8 \times 10^{19}$
Effective VB density ( $\text{cm}^{-3}$ )	$1.04 \times 10^{19}$	$1.04 \times 10^{19}$	$1.04 \times 10^{19}$
Electron velocity (cm/s)	$1.0 \times 10^7$	$1.0 \times 10^7$	$1.0 \times 10^7$
Hole velocity (cm/s)	$1.0 \times 10^7$	$1.0 \times 10^7$	$1.0 \times 10^7$
Electron mobility ( $\text{cm}^2/\text{Vs}$ )	1400	1400	1400
Hole mobility ( $\text{cm}^2/\text{Vs}$ )	450	450	450
Donor density ( $\text{cm}^{-3}$ )	$1.0 \times 10^{20}$	-	-
Acceptor density ( $\text{cm}^{-3}$ )	-	$1.0 \times 10^{16}$	$1.0 \times 10^{20}$
Defect density ( $\text{cm}^{-3}$ )	-	-	-

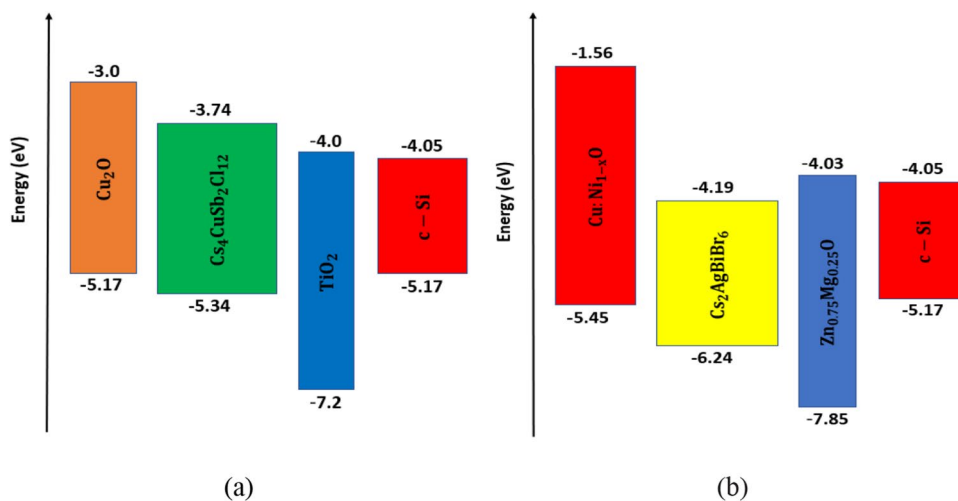
energy band structures. The minimum energy levels of VB (valence band) and CB (conduction band) in the EBD are represented by the lower and upper boundaries for each utilized materials, respectively. The refractive index (n) and extinction coefficient (k) of various layers in the top cells have been calculated using the methods outlined in the literature [32, 33] and are listed in Table 2 at a wavelength of 320 nm.

### 3 Device Design

In this work, numerical designs of lead-free double perovskite/c-Si TDs are implemented through the utilization of SCAPS-1D software, specifically version 3.3.10. This software relies on three fundamental semiconductor equations: Poisson's equation, hole and electron continuity equations, collectively elucidating the mechanisms of carrier generation

and recombination within device layers [34]. The optical and recombination models integrated into SCAPS are showcased in Table 5. The similarities between the simulated results from this software and the experimental findings reported in numerous literature works are evident. SCAPS-1D simulator does not entirely allow simulating a photovoltaic device featuring a multijunction configuration. In multijunction modelling, it is a frequent assumption that the tunnel junction is ideal. It is assumed that there are negligible optical and electrical losses at interfaces of considered TDs under the present study. The device models of standalone TCs and BC have initially been calibrated making use of existing experimental settings from literature, as detailed in Tables 2, 3 and 4. The performance parameters of calibrated models along with the results derived from the reported experimental observations, are mentioned and compared in Table 6. Figure 3 illustrates the J-V characteristics of the designed standalone device structures in comparison with published measurement. The obtained performance parameters follow the reported measurements [24, 25, 37]. By calibrating the standalone both the sub-cells, this study ensures high accuracy in reflecting the real values. Further optimization of absorber thickness is required to boost TC performance. For TC to perform better, absorber thickness needs to be further optimized. It is necessary to point out that parameter values are optimized for different layers except thickness of absorber layer and listed in Tables 2, 3 and 4. A tandem solar device's sub-cells can be considered a pair of series-connected diodes. While analyzing the performance of TDs, TC and BC are simulated separately to obtain current matching points. The J-V characteristics of TD are then determined by treating them as an equivalent series connection. The device design of TC (wide bandgap) is performed using AM1.5G solar spectrum, while BC (narrow bandgap) is designed utilizing a filtered spectrum derived from TC. The filtered/transmitted spectrum,  $S(\lambda)$  (from TC to BC) is calculated using Eq. (1) [30, 38]:

**Fig. 2** Illustration of EBDs for materials utilized in **a** TD-1, and **b** TD-2 configurations

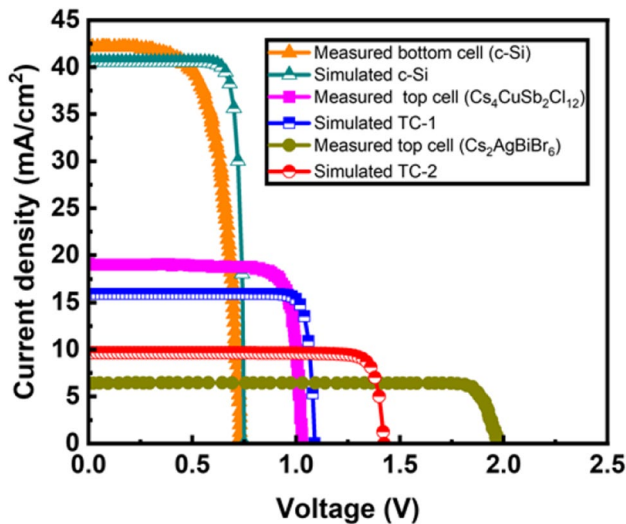


**Table 5** Optical and recombination models utilized in SCAPS simulation

Optical model	Recombination model
<p>The optical model utilized to compute generation of electron-hole (eh) pairs from incident photon flux comprises following equations [35]:</p> $N_{\text{phot}}(\lambda, x) = N_{\text{phot0}}(\lambda) \cdot T_{\text{front}}(\lambda) \cdot \exp(-x\alpha(\lambda)) \cdot \frac{1 + R_{\text{back}}(\lambda) \cdot \exp(-2(d-x)\alpha(\lambda))}{1 - R_{\text{back}}(\lambda) \cdot R_{\text{int}} \cdot \exp(-2d\alpha(\lambda))}$ $G(\lambda, x) = \alpha(\lambda, x) \cdot N_{\text{phot}}(\lambda, x)$ $G(x) = \int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} G(\lambda, x) d\lambda = \int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} \alpha(\lambda, x) \cdot N_{\text{phot}}(\lambda, x) d\lambda$ <p>Where, <math>N_{\text{phot}}(\lambda, x)</math> signifies the photon flux at each position in the layer, <math>N_{\text{phot0}}(\lambda)</math> denotes the incident photon flux, and at each wavelength, <math>T_{\text{front}}(\lambda)</math> represents the transmission of the front contact, <math>\alpha(\lambda)</math> stands for the absorption coefficient, <math>R_{\text{int}}</math> stands for the internal reflection at the front contact, <math>R_{\text{back}}</math> signifies the reflection at the back contact, <math>\lambda</math> represents wavelength, <math>d</math> represents the layer thickness, <math>x</math> represents the position in the layer, and <math>G(x)</math> denotes the generation rate of electron-hole pairs.</p>	<p>In SCAPS simulation, the introduction of three distinct recombination processes: Shockley-Read-Hall (SRH) recombination, radiative recombination, and Auger recombination is facilitated through the utilization of the following equations [34, 36]:</p> $R_{\text{SRH}} = \frac{np - n_i^2}{\tau_p(n + n_0) + \tau_n(p + p_0)}$ $R_{\text{radiative}} = K(np - n_i^2)$ $R_{\text{Auger}} = (C_n n + C_p p)(np - n_i^2)$ <p>Where, <math>R_{\text{SRH}}</math>, <math>R_{\text{radiative}}</math> and <math>R_{\text{Auger}}</math> denote the SRH, radiative, and Auger recombination rates, respectively, with <math>n</math> and <math>p</math> representing the concentrations of electrons and holes in the conduction and valence bands, <math>n_0</math> and <math>p_0</math> denoting the equilibrium concentrations, <math>\tau_n</math> and <math>\tau_p</math> signifying the lifetimes of electrons and holes, <math>n_i</math> representing intrinsic carrier concentration, and <math>K</math>, <math>C_n</math> and <math>C_p</math> are the radiative recombination coefficient, Auger electron and hole capture coefficients, respectively.</p>

**Table 6** Calibration of standalone TCs and BC using experimental parameters

Device structure	V <sub>OC</sub> (V)	J <sub>SC</sub> (mA/cm <sup>2</sup> )	FF (%)	PCE (%)	Reference/ID
n + Si/pSi/p + Si	0.74	42.30	83.8	26.35	[32]
n + Si/pSi/p + Si	0.75	40.52	85.25	26.09	c-Si
TiO <sub>2</sub> /Cs <sub>4</sub> CuSb <sub>2</sub> Cl <sub>12</sub> nanocrystals/Cu <sub>2</sub> O	1.03	19.07	82.01	16.11	[25]
TiO <sub>2</sub> /Cs <sub>4</sub> CuSb <sub>2</sub> Cl <sub>12</sub> /Cu <sub>2</sub> O	1.09	15.91	88.66	15.38	TC-1
SnO <sub>2</sub> /Cs <sub>2</sub> AgBiBr <sub>6</sub> /Cu <sub>2</sub> O	1.97	6.39	89.5	11.32	[24]
Zn <sub>0.75</sub> Mg <sub>0.25</sub> O/Cs <sub>2</sub> AgBiBr <sub>6</sub> /Cu : Ni <sub>1-x</sub> O	1.42	9.65	87.21	11.99	TC-2



**Fig. 3** J-V curves of standalone TCs and BC along with published measurements

$$S(\lambda) = S_0(\lambda) \cdot \exp\left(\sum_{i=1}^4 -\alpha_{\text{layer}_i}(\lambda) \cdot d_{\text{layer}_i}\right) \tag{1}$$

where  $S_0(\lambda)$  denotes AM 1.5G solar spectrum,  $\alpha(\lambda)$  represents absorption coefficient,  $\lambda$  signifies wavelength,  $d$  stands for thickness of the several layers in TC, and  $\text{layer}_i$  refers to a specific layer ( $i = 1$  corresponds to FTO, 2 to ETL, 3 to absorber, and 4 to HTL).  $\alpha(\lambda)$  for different layers of the TC are depicted in Fig. 4, which are used in Eq. (1). The current matching requirement is essential because inadequate current matching between TC and BC may result in an accumulation of surplus charge carriers at the recombination interface, negatively impacting recombination behavior [39]. Achieving current matching between the TC and BC in a tandem configuration involves fine-tuning of TC’s thickness to ensure that its current, generated under the AM1.5G solar spectrum, matches BC’s current under a filtered spectrum corresponding to TC. The minimal current obtained from TC and BC defines the tandem current’s value i.e., current matching point. This matching point can greatly boost the tandem cell’s performance. The two cells can generate more



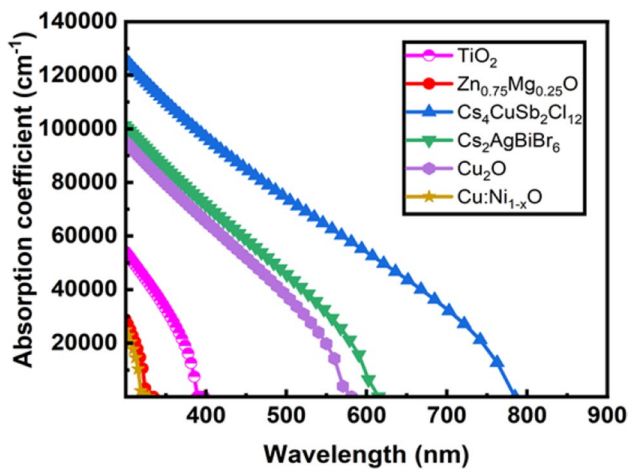


Fig. 4 Absorption coefficients of different layers of the TCs

current when this point is raised, contributing to an improvement in the overall PCE of TD.

## 4 Results and Discussion

A 2-T, TD is a series connection of a TC and a BC, as described in Section 3. Thus, TD's  $V_{OC}$  (open circuit voltage) is the total of its sub-cell voltages. However, the lowest value of junction currents will set a limit on the overall device's  $J_{SC}$  (short circuit current density). Device design results of standalone individual cells along with the overall TD are presented and explained in the following Section 4.1 to Section 4.3. For enhancing the overall performance of TD, extensive investigations have also been carried out to explore the performance of double perovskite based TCs. These investigations involve systematic variations of key parameters such as absorber thickness, doping density, defect density, and interface (ETL/absorber and absorber/HTL) defects in Section 4.2 (4.2.1–4.2.4). A comparison of the obtained results with

the recently reported results for the designed TDs is showcased in Section 4.5.

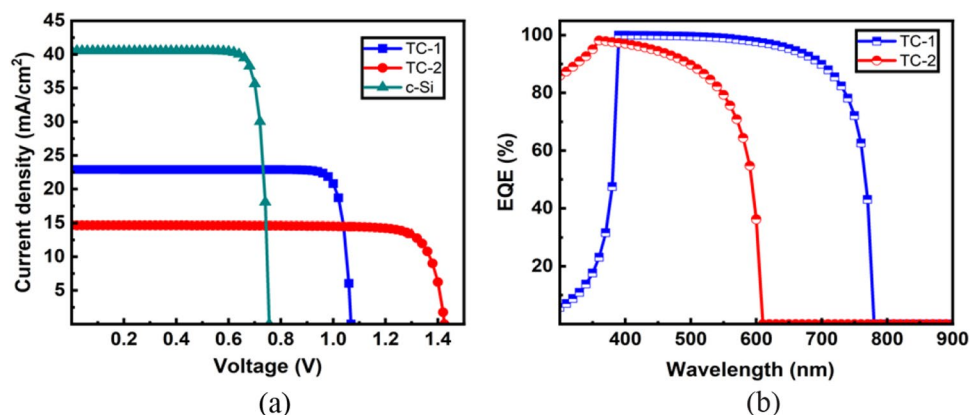
### 4.1 Standalone c-Si BC

In this study, both TD-1 and TD-2 feature a c-Si solar cell as their BC. The thickness values utilized for the n+ Si, p Si, and p+ Si layers are 0.2  $\mu\text{m}$ , 300  $\mu\text{m}$ , and 10  $\mu\text{m}$ , respectively. The device design of standalone c-Si cell is performed utilizing the AM1.5G solar spectrum, and the device model exhibits  $\text{PCE} = 26.09\%$ . ( $V_{OC} = 0.75$  V,  $J_{SC} = 42.52$   $\text{mA}/\text{cm}^2$  and  $\text{FF} = 85.25\%$ ). Table 5 presents the simulated and reported experimental values [37]. Figure 5a displays the BC's simulated J-V plot. The resulting performance parameters closely match the reported experimental values, providing the critical validation of the proposed methodology.

### 4.2 Standalone Lead-Free Double Perovskite TCs

In this work, two TCs made of  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  (TC-1) and  $\text{Cs}_2\text{AgBiBr}_6$  (TC-2) absorber layers have been utilized for TDs TD-1 and TD-2 respectively. Both TCs (with absorber layer thickness value of 0.2  $\mu\text{m}$ ) have been initially simulated under AM1.5G solar spectrum in standalone conditions. The performance parameters of the initial simulation along with the reported experimental results [24, 25] are mentioned and compared in Table 5. The obtained performance parameters agree well with the experimental values that have been published, which is a critical component for validation of proposed method. The results inspire confidence in moving forward with TD simulation. The thickness of the TC's absorber plays a pivotal role in augmenting performance in tandem design. At following thicknesses of various layers, TC's performance is further improved. The layer thicknesses for TC-1: 0.03  $\mu\text{m}$ , 0.7  $\mu\text{m}$  and 0.2  $\mu\text{m}$  of  $\text{TiO}_2$  (ETL),  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  (absorber layer) and  $\text{Cu}_2\text{O}$  (HTL) respectively. The layer thicknesses for TC-2: 0.03  $\mu\text{m}$ , 0.5  $\mu\text{m}$  and 0.098  $\mu\text{m}$  of  $\text{Zn}_{0.75}\text{Mg}_{0.25}\text{O}$  (ETL),  $\text{Cs}_2\text{AgBiBr}_6$  (absorber layer) and  $\text{Cu}:\text{Ni}_{1-x}\text{O}$  with  $\text{Cu}:\text{Ni}:\text{O}$

Fig. 5 a J-V plots of standalone TCs and BC, and b EQE plots of the standalone TCs



ratio of 0.14:0.68:1 (HTL) respectively. The TC-1 and TC-2 cell models exhibit PCE of 21.49% ( $V_{OC} = 1.07$  V,  $J_{SC} = 22.90$  mA/cm<sup>2</sup>, and FF = 87.80%), and 17.48% ( $V_{OC} = 1.42$  V,  $J_{SC} = 14.65$  mA/cm<sup>2</sup>, and FF = 83.69%) respectively. Figure 5a depicts the simulated J-V curves, while b depicts external quantum efficiency (EQE) curves for both standalone TCs. At a wavelength of 380 nm, TC-2 achieves more than 90% EQE, which then drops to below 65% at wavelengths over 580 nm. When compared to TC-1, TC-2 achieves more than 90% EQE at a lower wavelength. This is a result of the absorber layer of TC-2 having a high bandgap (2.05 eV). As evident from Fig. 5b, the EQE cut-off wavelength is 30% longer in TC-1, resulting in a higher  $J_{SC}$ . The simulated EQE value for the TC-2 follows the experimentally measured EQE [30, 40]. Furthermore, the performance of TCs has been investigated by tuning absorber layer as well as interface parameters.

#### 4.2.1 Impact of Tuning Absorber's Thickness

The performance analysis of TCs involves investigating the influence of varying the absorber layer's thickness, ranging from 0.2 to 2  $\mu\text{m}$ . Figure 6a–d illustrate the changes in performance parameters ( $V_{OC}$ ,  $J_{SC}$ , FF, and PCE) with respect to the absorber's thickness. A thin absorber results in poor recombination and a high  $V_{OC}$ . It is noticeable that  $J_{SC}$  value rises in both cells with the augmentation of the absorber's thickness. This enhancement can be attributed to the amplified absorption of incident photons and a greater number of electron-hole pairs generated. However, beyond a certain thickness, the PCE exhibits a decline. This decrease is associated with the heightened occurrence of recombination processes (radiative, Shockley-Read-Hall, and Auger recombinations) within the absorber material as a result of the thicker layers. Increasing absorber thickness improves carrier generation rate, enhancing efficiency with elevated  $J_{SC}$  but also increases recombination rates as carriers cover longer distances, impacting device's performance [41, 42]. These findings highlight the importance of optimizing the absorber layer's thickness to strike a balance between photon absorption (generation rate) and recombination rate, ultimately maximizing the PCE of TCs. The generation and recombination profiles are acquired and presented in Fig. 7a–d, confirming the increased penetration of these rates within the absorber at greater thicknesses. With the optimized thicknesses set at 1.2 and 1.5  $\mu\text{m}$ , TC-1 and TC-2 have attained PCE values of 21.99% and 22.56%, respectively.

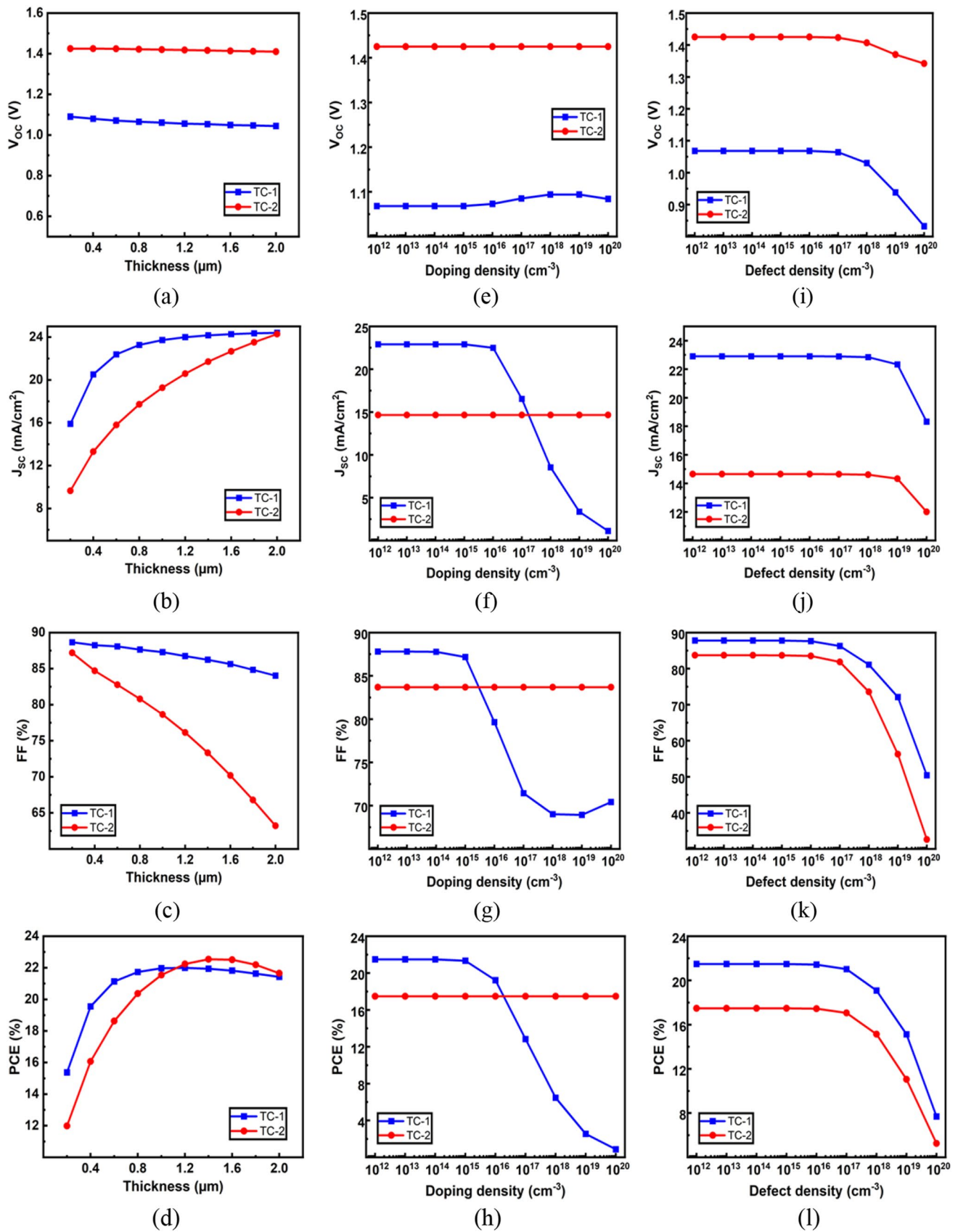
#### 4.2.2 Impact of Tuning Absorber's Doping Density

The doping density in absorber layer has been tuned from  $10^{12}$  to  $10^{20}$  cm<sup>-3</sup> for both cells to see how it affects the performance of the device. Figure 6e–h depict the change in performance parameters with varying doping density of absorber. From Fig. 6e–h, it is evident that the changes in performance parameters are minimal when the doping density changes for TC-2, while PCE declines with increasing doping density after its value of  $10^{13}$  cm<sup>-3</sup> for TC-1. The device's overall performance remains relatively stable at lower doping densities, but deteriorates at higher doping densities. The selected values for doping density that yield optimal performance in TC-1 and TC-2 are  $10^{13}$  and  $10^{16}$  cm<sup>-3</sup>, which exhibit PCE of 21.49% and 17.48%, respectively. To gain a better insight into the impact of doping concentration on performance parameters, the generation and recombination rates are depicted with position in Fig. 7e–h. It is noteworthy that the generation rate shows consistency across various doping levels. Higher doping concentration raises the electric field at absorber interface, improving the separation process but adversely impacting performance due to increased recombination [36, 43].

This demonstrates how improving device performance requires correct doping in the absorber material.

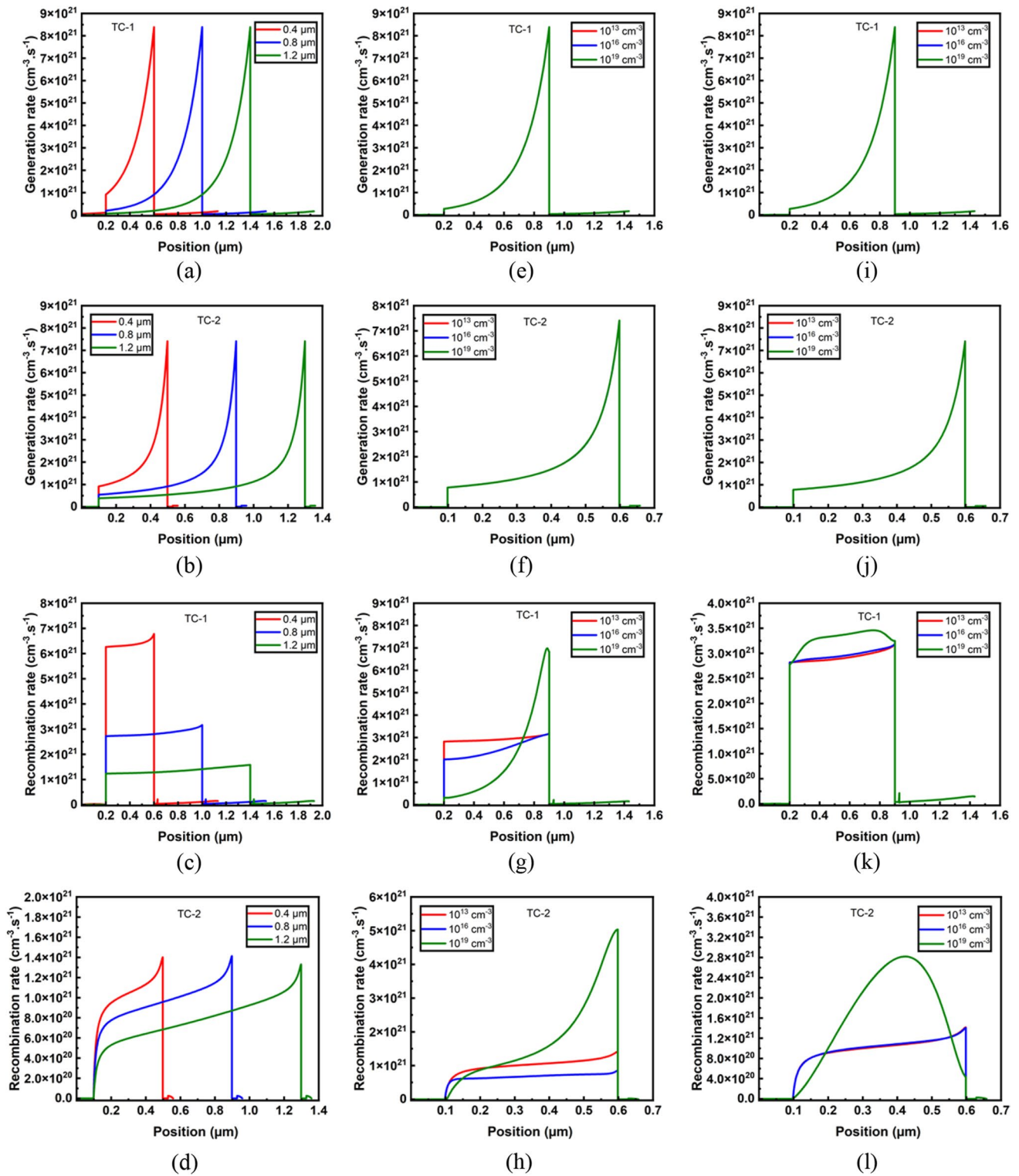
#### 4.2.3 Impact of Tuning Absorber's Defect Density

Increasing defect density results in more point defects in absorber layer, resulting in higher recombination. The lifetime of carriers decreases with more recombination. A rise in recombination diminishes the performance parameters of the device. Experimental methods for calculating these properties include intensity-modulated photovoltage, along with terahertz spectroscopy [44]. To investigate the impact of defect density in absorber layer on device performance, it is changed from  $10^{12}$  to  $10^{20}$  cm<sup>-3</sup>. PCE for TC-1 and TC-2 decreases by 29.6% and 36.78%, respectively, when defect density increases from  $10^{15}$  to  $10^{19}$  cm<sup>-3</sup>. This is due to the elevated possibility of recombination as the defect density increases. Figure 6i–l show how performance parameters changed with varying absorber defect densities. The optimum values of defect density are taken for TC-1 and TC-2 are  $10^{13}$  and  $10^{15}$  cm<sup>-3</sup>, which exhibit PCE of 21.49% and 17.48%, respectively. The analysis of Fig. 6i–l indicates a clear inference that an increase in the defects within the absorber results in a decline in performance parameters. Additionally, Fig. 7i–l portrays the profiles of generation and recombination rates across

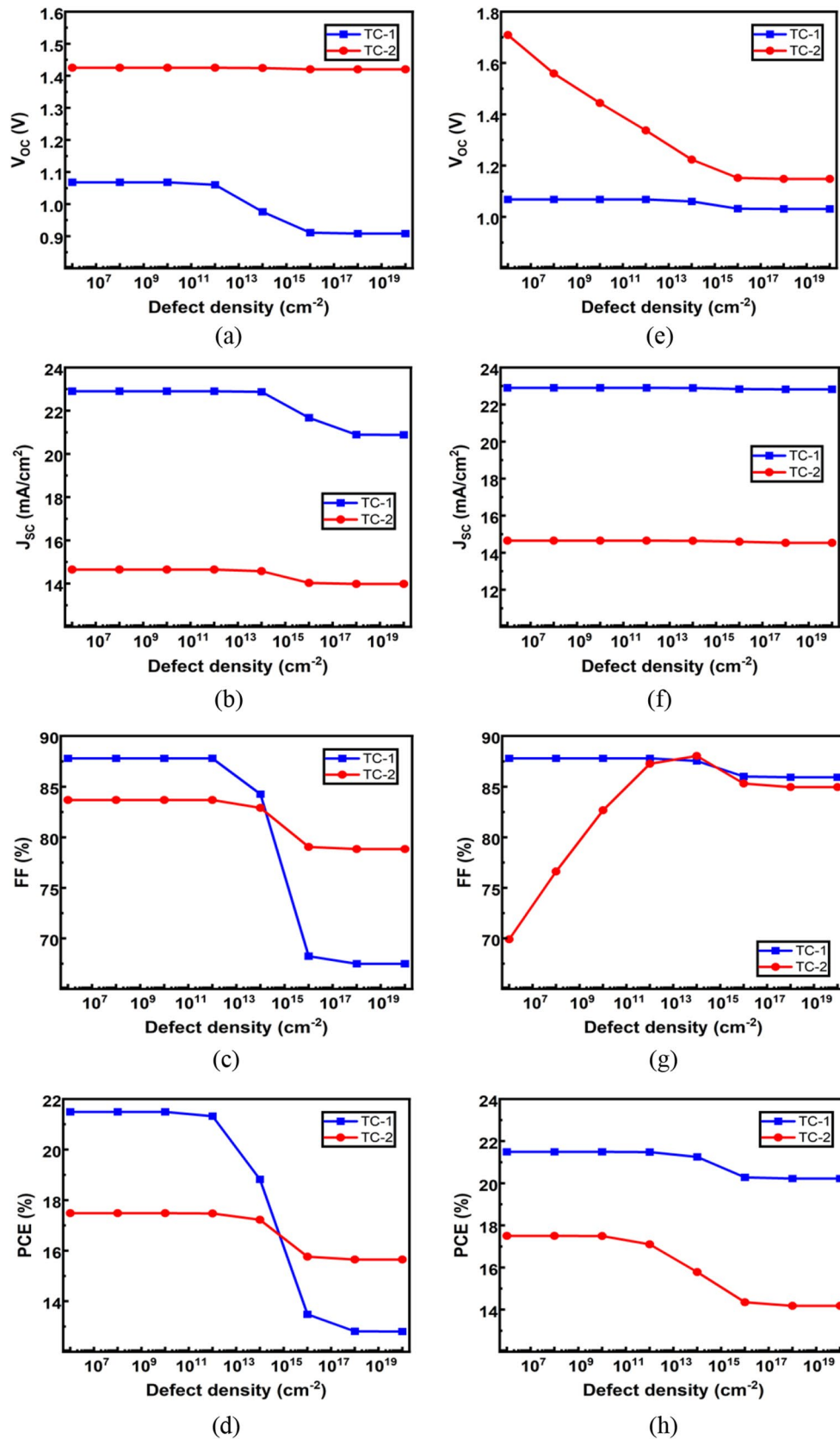


**Fig. 6** TC's performance parameters in relation to tuning absorber thickness (a–d), doping density (e–h), and defect density (i–l)





**Fig. 7** TC's carrier generation and recombination rate profiles for different values of absorber thickness (a–d), doping density (e–h), and defect density (i–l)



**Fig. 8** TC's performance parameters in relation to tuning defect density at ETL/absorber (a–d), and absorber/HTL (e–h) interfaces

different defect density values. Notably, the generation rate exhibits stability across varying doping levels. Figure 7k–l highlights the notable influence of defect density on the absorber layer's recombination rate, resulting in increased carrier recombination with higher defect density. As a consequence, there is a reduction in carrier lifetime and diffusion length, contributing to the overall decline in device performance [41, 45].

#### 4.2.4 Impact of Tuning Interface's Defect Density

Reducing carrier recombination within the interface is significant to enhance carrier extraction. The ETL/absorber and absorber/HTL interface defects are varied between  $10^6$  to  $10^{20}$  cm<sup>-2</sup> to investigate their impact on device performance. The impact of interface defects on TC's performance is clearly illustrated in Fig. 8a–h. Device performance for both cells remain unchanged by ETL/absorber interface defect density below  $10^{10}$  cm<sup>-2</sup>, while PCE values for TC-1 and TC-2 decrease by 40.39% and 10.46%, respectively, with a rise in defect levels from  $10^{10}$  to  $10^{18}$  cm<sup>-2</sup>. Device performance for both cells remain unchanged by absorber/HTL interface defect level below  $10^{12}$  cm<sup>-2</sup>, while PCE values for TC-1 and TC-2 decrease by 5.86% and 17.07%, respectively, with a rise in defect density from  $10^{12}$  to  $10^{18}$  cm<sup>-2</sup>.

#### 4.3 Lead-Free Double Perovskite/c-Si TSCs

In order to simulate double perovskite/c-Si TSCs (TDs), a fairly straightforward approach is being adopted. The method for simulating the TD has been explained in Section 3. Due to the fact that sub-cells of a TD can be conceptualized as a pair of diodes electrically coupled in series, ensuring current matching between them is essential. At current matching point, TC and BC possess identical  $J_{SC}$  or  $J_{MP}$  (current density corresponding to maximum power point) values. The cell having lower  $J_{SC}$  value determines the total  $J_{SC}$ , and addition of sub-cell's  $V_{OC}$  values provides total  $V_{OC}$  for the TDs. Two TDs, TD-1 (TC-1/c-Si) and TD-2 (TC-2/c-Si), have been designed and simulated in this study. The device design of TCs (TC-1 and TC-2) is performed using AM1.5G spectrum, while BC simulation is performed using a filtered spectrum generating through TC. To achieve current matching among sub-cells, TC's absorber thickness is finely adjusted. This tuning process ensures that the TC's current (when exposed to the AM1.5G spectrum), matches the BC's current (generated in the presence of a filtered spectrum). At first, thickness of absorber layer of TC-1 and TC-2 was changed from 0.2 to 2  $\mu$ m, while thicknesses of the other layers remained fixed. For each value of absorber thickness, a specific filtered spectrum was obtained. Subsequently, this filtered spectrum was employed to illuminate the BC. In Fig. 9, the variations in

$J_{SC}$  and  $J_{MP}$  values for both the TC and BC are shown as a function of TC's absorber thicknesses. Analysis of Fig. 9 reveals a notable similarity in the trends exhibited by  $J_{SC}$  and  $J_{MP}$ , indicating a consistent behavior in the underlying device physics. For TD-1,  $J_{SC}$  and  $J_{MP}$  current matching conditions have been obtained at TC-1's absorber thickness values, 0.418 and 0.41  $\mu$ m, respectively. For TD-2,  $J_{SC}$  and  $J_{MP}$  current matching conditions have been obtained at TC-2's absorber thickness values, 1.29 and 1.41  $\mu$ m, respectively. In Fig. 10, the AM 1.5G spectrum is depicted as the illumination source for TCs, and the filtered spectra (under the conditions of  $J_{SC}$  current matching) are shown, utilized in illuminating the BC. With the above  $J_{SC}$  matching conditions, lead-free double perovskite/c-Si TDs (TD-1 and TD-2) have been simulated. The resulting J-V plots are presented in Fig. 11, and Table 6 details the performance parameters for the TDs. The TD-1 and TD-2 exhibit PCE of 34.67% (with  $V_{OC}$  = 1.82 V,  $J_{SC}$  = 20.75 mA/cm<sup>2</sup>, FF = 88.31%), and 36.88% (with  $V_{OC}$  = 2.16 V,  $J_{SC}$  = 21.105 mA/cm<sup>2</sup>, FF = 79.68%), respectively.  $J_{SC}$  values for TD-1 and TD-2 are interestingly comparable. The  $V_{OC}$  and PCE values of TD-2 are higher as compared to TD-1, likely due to the larger thickness and bandgap values of Cs<sub>2</sub>AgBiBr<sub>6</sub> compared with Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub>. Table 7; Fig. 10 make evident that BC (lower  $J_{SC}$ ) limits the TD's total  $J_{SC}$ , and the addition of  $V_{OC}$  values of each sub-cell provide the total  $V_{OC}$  for both TD-1 and TD-2.

#### 4.4 Comparison with the Recently Reported Results

The comparison of this work with recently reported experimental and simulated results of TDs is shown in Table 8. Performance metrics, including  $V_{OC}$ ,  $J_{SC}$ , FF, and PCE of TDs obtained from this work are comparable to those of the reported experimental and simulated devices [2, 30, 38, 46–49]. The results of this work show that lead-free double perovskite/c-Si TDs can theoretically achieve PCE exceeding 36.88% (TD-2). With regard to performance, this TD structure is an intriguing substitute for conventional silicon solar cells, that offers higher efficiency, better stability, and less expensive manufacturing.

### 5 Conclusions

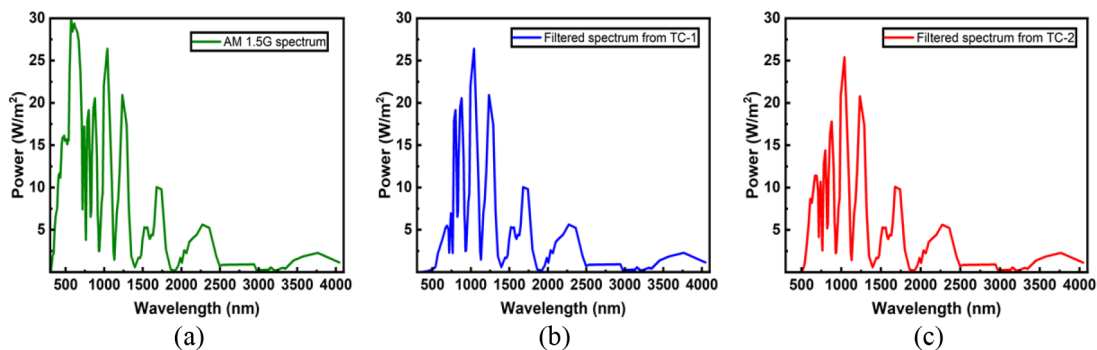
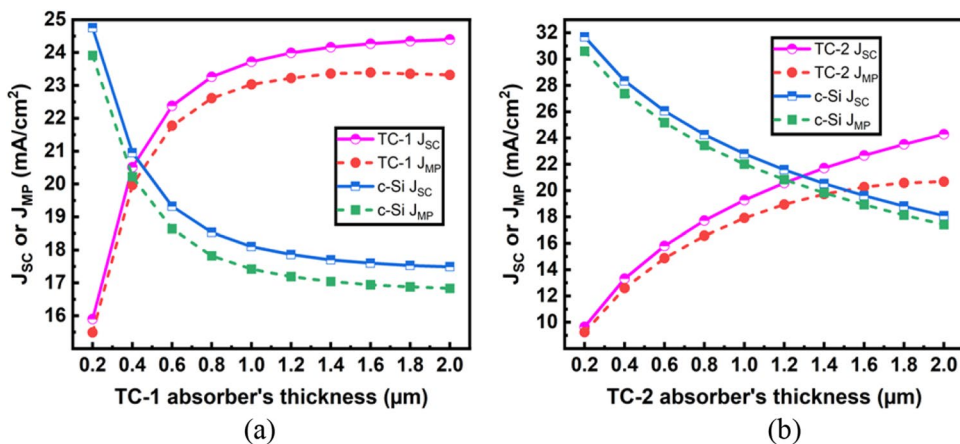
This study involves the design and exploration of lead-free TDs incorporating double perovskite/ c-Si structures using SCAPS 1-D. Two lead-free double perovskite materials, Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub> and Cs<sub>2</sub>AgBiBr<sub>6</sub> have been investigated as the absorber materials for TCs, while the BC comprises a c-Si photovoltaic cell. In order to devise an efficient TD structure, a stepwise approach was followed: initially, standalone device designs were done for both TC and BC, after which

**Table 7** Performance parameters of TDs, including their respective TC and BC

Cell	$V_{oc}$ (V)	$J_{sc}$ (mA/cm <sup>2</sup> )	FF (%)	PCE (%)
TC-1	1.08	20.755	88.23	19.77
c-Si (filtered)	0.74	20.750	85.23	25.61
TD-1 (TC-1/c-Si)	1.82	20.750	88.31	34.67
TC-2	1.42	21.109	74.92	22.42
c-Si (filtered)	0.74	21.105	85.23	25.30
TD-2 (TC-2/c-Si)	2.16	21.105	79.68	36.88

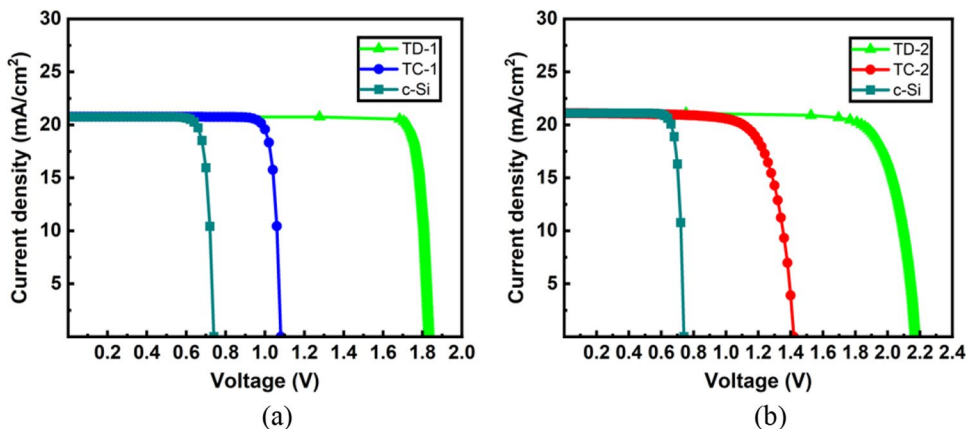
they were coupled in series. To achieve optimal performance, particular attention was given to achieving a current matching condition between sub-cells. This was accomplished by finely tuning the absorber layer thickness of TC until the current generated under AM 1.5G spectrum matched the BC’s current obtained under the filtered spectrum specific to the TC’s absorption characteristics. After reaching the condition of current matching, the optimized thickness for Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub> and Cs<sub>2</sub>AgBiBr<sub>6</sub> layers are 0.418 and 1.29 μm, respectively. The lead-free Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub>/c – Si

**Fig. 9**  $J_{sc}$  and  $J_{MP}$  values of the TC and BC plotted against TC’s absorber thicknesses for a TD-1, and b TD-2



**Fig. 10** a AM 1.5G spectrum illuminated on the TCs, b and c filtered spectrum (under  $J_{sc}$  current matching conditions) illuminated on the BC transmitted from TC-1 and TC-2

**Fig. 11** J-V plots of a TD-1 and b TD-2, along with their respective TC and BC characteristics





**Table 8** Comparison of TD's performance with reported experimental and simulated results

TD (TC/BC)	$V_{OC}$ (V)	$J_{SC}$ (mA/cm <sup>2</sup> )	FF (%)	PCE (%)	Reference/ID	Year	Type of Analysis
Perovskite/Si	1.82	17.44	75.80	24.06	[50]	2023	Exp.
Perovskite/Si	1.75	16.36	80.33	23.00	[51]	2023	Exp.
Perovskite/Si	1.88	20.26	77.30	29.50	[2]	2022	Exp.
Perovskite/Si	1.80	18.81	77.50	26.30	[46]	2020	Exp.
Perovskite/Si	1.90	19.23	79.40	29.15	[47]	2020	Exp.
GaInP/Si	2.07	17.04	88.00	31.10	[48]	2020	Exp.
Perovskite/Si	2.30	17.52	67.39	27.25	[52]	2023	Sim.
Perovskite/SnS	1.99	16.99	85.15	28.92	[38]	2022	Sim.
Perovskite/Si	1.87	20.3	84.70	32.20	[49]	2021	Sim.
Perovskite/Si	1.76	16.01	86.70	24.40	[30]	2021	Sim.
Lead-free double perovskite/c-Si	1.82	20.75	88.31	34.67	TD-2	<i>This work</i>	Sim.
Lead-free double perovskite/c-Si	2.16	21.10	79.68	36.88	TD-2	<i>This work</i>	Sim.

Exp. Experimental, Sim. Simulation

and Cs<sub>2</sub>AgBiBr<sub>6</sub>/c – Si TDs exhibits a PCE of 34.67% (with  $V_{OC}$  = 1.82 V,  $J_{SC}$  = 20.75 mA/cm<sup>2</sup>, FF = 88.31%) and 36.88% (with  $V_{OC}$  = 2.16 V,  $J_{SC}$  = 21.105 mA/cm<sup>2</sup>, FF = 79.68%), respectively.  $J_{SC}$  values for both the devices are interestingly comparable. The  $V_{OC}$  and PCE values of Cs<sub>2</sub>AgBiBr<sub>6</sub>/c – Si TD are higher as compared to Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub>/c – Si TD, likely due to the greater thickness and bandgap values of Cs<sub>2</sub>AgBiBr<sub>6</sub> compared with Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub>. Analysis of this study implies that enhancing the performance of double-perovskite TC is required to realize the overall benefits of the TD. The results reported here demonstrate that lead-free and stable double perovskite materials can act as an important absorber of sub-cell for highly efficient, commercially viable, non-toxic and eco-friendly tandem photovoltaic technologies. The insights derived from this device design study will aid researchers in designing and fabricating TDs with improved device performance for the real time photovoltaic applications.

**Acknowledgements** Authors are grateful to the Department of Science and Technology (DST), Govt. of India, for financial backing through DST SERB Project File No. SRG/2021/002110. Dr. Amitesh Kumar acknowledges DST SERB regarding the Start-up Research Grant, fostering research at NIT Patna. Mr. Pritam Kumar expresses gratitude for providing and supporting facilities for research extended by the Department of Electrical Engineering, NIT Patna. Prof. Marc Burgelman from the University of Gent, Belgium, is appreciated for providing the crucial open-source SCAPS-1D software essential to this work.

**Author Contributions** PK: Conceptualization, Methodology, Visualization, Investigation, Data curation, Software, Writing-original draft. AK: Conceptualization, Methodology, Formal analysis, Supervision, Reviewing and Editing.

**Funding** Authors are grateful to the Department of Science and Technology (DST), Govt. of India, for financial backing through DST SERB Project File No. SRG/2021/002110.

**Data Availability** No datasets were generated or analysed during the current study.

## Declarations

**Ethical Approval** Not applicable.

**Competing Interests** The authors declare no competing interests.

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