

Numerical simulation of Cs₂TiBr₆-based all-inorganic photovoltaic perovskite solar cell employing SCAPS-1D software

P. R. Jubu^{a,b}, A. D. Otor^c, A. N. Abutu^b, A. O. Aransiola^{a,d}, C. Amakom^{a,e}, K. I. Udofia^{a,f}, I. K. Nwokolo^a, A. A. Goje^{a,g}, I. I. Ayogu^a, M. M. Gururani^h, E. E. Oguzie^{a,i,*}

^aAfrica Centre of Excellence in Future Energies and Electrochemical Systems (ACE-FUELS), Federal University of Technology Owerri (FUTO), P.M.B. 1526 Owerri, Imo State, Nigeria

^bDepartment of Industrial Physics, Joseph Sarwuan Tarka University Makurdi (Federal University of Agriculture Makurdi), P.M.B. 2373, Makurdi, Benue State, Nigeria

^cDepartment of Physics, Joseph Sarwuan Tarka University Makurdi (Federal University of Agriculture Makurdi), P.M.B. 2373, Makurdi, Benue State, Nigeria

^dDepartment of Electronic and Electrical Engineering, Obafemi Awolowo University, Ile-Ife, Nigeria

^eDepartment of Physics, Federal University of Technology Owerri (FUTO), P.M.B. 1526 Owerri, Imo State, Nigeria

^fDepartment of Physics, Akwa Ibom State University, Akwa Ibom State, Nigeria

^gDepartment of Applied Physics, Federal Polytechnic Damaturu, Nigeria

^hDepartment of Physics, M.B. Government P.G. College, Haldwani, Uttarakhand, India

ⁱDepartment of Chemistry, Federal University of Technology Owerri (FUTO), P.M.B. 1526 Owerri, Imo State, Nigeria

Abstract

Lead halide perovskite solar cells (PSCs) show considerable promise, but their inherent drawbacks, including low stability and toxicity, pose environmental concerns. Therefore, exploring lead-free perovskite materials as potential alternative absorber layers is imperative. This work investigates a Cs₂TiBr₆/CZTSe photoactive heterostructure in which Cs₂TiBr₆ serves as the primary wide-bandgap absorber while CZTSe provides additional near-infrared absorption and hole transport. Numerical simulation is an effective way to identify suitable materials and device architectures for efficient photovoltaic systems, and it reduces fabrication costs and material wastage arising from extensive experimental trials. The SCAPS-1D software was employed to propose the FTO/CeO_x/Cs₂TiBr₆/CZTSe/CuO/Pt electron transport layer-assisted (ETL-assisted) PSC, which delivered a high power conversion efficiency (PCE) of 27.12% after optimization of structural parameters. Results show an increase in PCE from 27.12% to 36.10% with increasing sunlight concentration from 1 to 50 suns. Comparatively, the optimized ETL-free counterpart design, FTO/Cs₂TiBr₆/CZTSe/CuO/Pt, yielded a comparable and slightly higher PCE of 27.14%. This ETL-free design represents a first attempt for the Cs₂TiBr₆-based perovskite absorber and provides a strategy for reducing fabrication cost and device complexity associated with multistack configurations.

DOI: [10.46481/jnsps.2026.3366](https://doi.org/10.46481/jnsps.2026.3366)

Keywords: Cs₂TiBr₆ perovskite, ETL-free perovskite solar cell, SCAPS-1D, CZTSe, Power conversion efficiency

Article history:

Received: 18 March 2026

Received in revised form: 10 June 2026

Accepted for publication: 13 June 2026

Available online: 15 July 2026

© 2026 The Author(s). Published by the Nigerian Society of Physical Sciences under the terms of the Creative Commons Attribution 4.0 International license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

Communicated by: B. J. Falaye

1. Introduction

The increase in global warming caused by fossil-fuel combustion and environmental pollution by harmful chemicals calls

*Corresponding author Tel. No.: +2348037026581;

Email address: emeka.oguzie@futo.edu.ng (E. E. Oguzie)

for green technologies to mitigate these challenges [1, 2]. The green technologies for energy include, photoelectrochemical water splitting for hydrogen fuel production [2–4], photovoltaic (PV) solar cell [5, 6], bioenergy, wind energy, technologies, and geothermal energy technologies [7]. The PV technology is distinguished within green energy technologies due to its ability to convert sunlight directly into electricity without the need for fuel, mechanical components, or greenhouse gas emissions, leading to a clean and quiet operation. It provides significant scalability, ranging from compact portable systems to extensive utility-scale power plants, and can be utilized in various settings. Furthermore, PV technology enjoys swift cost reductions, extended operational lifespans, and ongoing enhancements in efficiency, positioning it as one of the most accessible and economically viable renewable energy options globally.

PSCs are gaining attention as possible alternatives to silicon-based cells because of their high power conversion efficiency (PCE) up to 26.20% derived from experiment [5], economical solution processing, adjustable bandgap, and suitability for lightweight and flexible substrates [8]. Cesium titanium hexabromide (Cs_2TiBr_6) is an excellent perovskite absorber for solar cells due to its lead-free composition, an appropriate bandgap of approximately 1.8–1.9 eV for the absorption of visible light, notable environmental stability, and the facilitation of efficient charge transport [9, 10]. Chen *et al.* (2018) first reported an experimental PCE of 3.3% for the Cs_2TiX_6 perovskite [11]. This effort stimulated interest in PSCs utilizing Cs_2TiBr_6 due to their lead-free composition and favorable optoelectronic characteristics [9, 10]. A handful of theoretical investigations on the Cs_2TiX_6 absorber can be found in the literature. Karmaker *et al.* reported a PCE of 26.96% using CuSbS_2 and ZnO as carrier transport materials (CTMs) [12], Gupta *et al.* obtained a PCE of 24.24% using SnO_2 and CBTS as CTMs [9], Hossain *et al.* achieved a PCE of 24.82% using La-doped BaSnO_3 and CNTS as CTMs [13], Mercy *et al.* got a PCE of 23.77% using CdS and Cu_2SbS_2 as CTMs [14], Lin *et al.*, recorded a PCE of 22.61% employing CeO_x , CZTS and P_3HT as CTMs [10], Urmi *et al.*, obtained a PCE of 21.17% employing TiO_2 and CuI as CTMs [15], and Kaur *et al.*, recorded a PCE of 20.11% using SnO_2 and MoO_x as CTMs [16].

Numerical simulation serves as an effective method for determining the best materials and device structure for advanced photovoltaic devices, greatly reducing production expenses and material waste that result from extensive experimental trials [17–19]. The current work proposes a modified solar cell configuration for the Cs_2TiX_6 perovskite absorber. CTMs such as CeO_x , CZTSe and CuO are employed to construct the $\text{FTO/CeO}_x/\text{Cs}_2\text{TiBr}_6/\text{CZTSe/CuO/Ni}$ PSC. The CeO_x electron transport layer (ETL) and the CZTSe/ CuO double hole transport layers (HTLs) are essential for enhancing the performance of the device. The CeO_x ETL, characterized by its wide bandgap, high electron mobility, and suitable conduction band alignment, enables efficient electron extraction from the absorber while preventing hole passage [10]. This helps to reduce front-interface recombination. The CZTSe/ CuO double HTLs offer high hole mobility and optimal valence band alignment with Cs_2TiBr_6 , which facilitates effective hole trans-

port and minimizes back-interface recombination [20, 21]. Together, this configuration of CTMs guarantees selective charge extraction, and mitigates recombination losses to enhance PV performance. It should be noted that in addition to its role as a hole transport material, the CZTSe possesses a narrow bandgap (~ 1.0 eV) and strong absorption extending into the near-infrared region. Therefore, when incorporated adjacent to the Cs_2TiBr_6 perovskite layer, CZTSe may contribute to photocarrier generation in addition to charge transport. This raises the possibility of a photoactive $\text{Cs}_2\text{TiBr}_6/\text{CZTSe}$ heterostructure in which both materials participate in solar energy conversion.

The new $\text{FTO/CeO}_x/\text{Cs}_2\text{TiBr}_6/\text{CZTSe/CuO/Ni}$ ETL-assisted design is investigated under varying layer thickness, bulk and interface defect density, back contact work function, and doping concentration of the CZTSe and CuO HTLs. Also, the effect of sun concentration on performance of the optimized device is also investigated. Furthermore, the ETL-free counterpart design of the optimized cell is investigated to understand the possibility of having an efficient cell without using an ETL. Excluding the ETL is an excellent strategy to achieve a simple and cost-effective design. This proposed ETL-free PSC architecture serves as a first-time attempt for the Cs_2TiBr_6 perovskite

2. Numerical simulation

To explore how well PSCs perform, researchers often employ various simulation programs like wxAMPS, COMSOL Multiphysics, SILVACO ATLAS, SCAPS-1D and the finite element method, among others. In this study, we chose SCAPS-1D because its simulation results often align well with practical experience [22]. We utilized SCAPS-1D software (version 3.3.0.7, developed from the University of Gent, Belgium) as our simulation platform for Cs_2TiBr_6 -based PSCs. This software is designed to solve the essential equations that describe charge transport in semiconductors within a one-dimensional framework. The Poisson equation, which illustrates the connection between electrostatic potential and charge density in one dimension, is expressed by (1) [23–25].

$$\frac{dE(x)}{dx} = \frac{d^2V(x)}{dx^2} = \frac{q}{\epsilon} [p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)], \quad (1)$$

where E is the electric field, ϵ is dielectric constant of the semiconductor equal to $\epsilon = \epsilon_r \epsilon_0$, where ϵ_r is the relative permittivity and ϵ_0 is vacuum permittivity, q is electron charge, N_A^- and N_D^+ are acceptor and donor carrier density, respectively, V is the electrostatic potential, p and n are the hole and electron concentration, n_t and p_t are the trapped electron and hole concentration, respectively, and x denote the position coordinate.

The continuity equations for holes (2) and electrons (3) can be written as:

$$\frac{dp_n}{dt} = G_p - \frac{p_n - p_{n0}}{\tau_p} + p_n \mu_p \frac{dE}{dx} + \mu_p E \frac{dp_n}{dx} + D_p \frac{d^2 p_n}{dx^2}, \quad (2)$$

$$\frac{dn_p}{dt} = G_n - \frac{n_p - n_{p0}}{\tau_n} + n_p \mu_n \frac{dE}{dx} + \mu_n E \frac{dn_p}{dx} + D_n \frac{d^2 n_p}{dx^2}, \quad (3)$$

where G_p and G_n denote the hole and electron generation rates, D_p and D_n represent the hole and electron diffusion coefficients expressed by the Einstein relation (4). The drift and diffusion equations for electrons and holes, which represent the carrier transport can be expressed in terms of the quasi-Fermi level, according to (5), (6).

$$D_i = \left(\frac{kT}{q} \mu_i \right), \quad (4)$$

$$J_n(x) = qn\mu_n E + qD_n n \frac{dn}{dx} = n\mu_n \frac{dE_{Fn}}{dx}, \quad (5)$$

$$J_p(x) = qp\mu_p E - qD_p p \frac{dp}{dx} = p\mu_p \frac{dE_{Fp}}{dx}, \quad (6)$$

where J_n and J_p are current density of electrons and holes, where E_F represent the quasi-Fermi levels, the subscripts p and n denote holes and electrons, respectively, μ_p and μ_n denote the hole and electron mobilities.

2.1. Device structure and rationale

Two prototype PSCs with single HTLs (FTO/CeO_x/Cs₂TiBr₆/CZTSe/Ni and FTO/CeO_x/Cs₂TiBr₆/CuO/Ni), and one PSC with double HTL (FTO/CeO_x/Cs₂TiBr₆/CZTSe/CuO/Ni) were constructed. A typical illustration of the dual HTL device is depicted in Figure 1a. Each device followed a multilayer heterojunction architecture where light illuminated through the FTO front electrode and transmitted to the Cs₂TiBr₆/CZTSe dual photoactive layer. The CeO_x served as the ETL due to its high band gap (3.5 eV), suitable electron affinity (4.4 eV), and decent electron mobility (100 cm²/V.s) [10]. CZTSe (Cu₂ZnSnSe₄) and CuO played the role of HTLs or back contact buffer layers to facilitate hole extraction and suppress recombination at the back contact. The dual HTL-based structure (CZTSe/CuO) aimed to integrate the strong hole conductivity of CuO with the favorable band alignment and reduced interface recombination provided by CZTSe, where the CZTSe layer plays dual roles of hole carrier transport and secondary absorber layer to assist in carrier generation. Figure 1b illustrates the energy level diagrams of the materials employed in this study.

2.2. Device simulation parameters

Table 1 shows the fundamental physical parameters of various materials extracted from relevant published studies [10, 23, 26, 27]. To simplify understanding and comparison, the thicknesses of all layers in all the three devices were kept the same during the prototype simulations. The parameters for the various interfaces can be found in Table 2. The work functions for

Table 1: Fundamental physical parameters employed for the study [10, 20, 21, 24, 25].

Parameter	Layer				
	FTO	CeO _x	Cs ₂ TiBr ₆	CZTSe	CuO
	[10]	[10]	[10]	[13, 20]	[26]
Thickness (μm)	0.5	0.1	0.4	0.1	0.2
E_g (eV)	3.5	3.5	1.8	1.0	1.51
χ (eV)	4.3	4.4	4.47	4.5	4.07
ϵ_r	9.0	9.0	10.0	13.6	18.1
N_C (cm ⁻³)	2.2×10^{18}	1.0×10^{20}	6.0×10^{19}	2.2×10^{18}	2.2×10^{19}
N_V (cm ⁻³)	1.8×10^{19}	2.0×10^{21}	2.0×10^{19}	1.8×10^{19}	5.5×10^{20}
μ_n (cm ² V ⁻¹ s ⁻¹)	200	100	4.4	20.0	100
μ_p (cm ² V ⁻¹ s ⁻¹)	10.0	25.0	2.5	10.0	0.1
$e V_{th}$ (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
$h V_{th}$ (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
N_D (cm ⁻³)	2×10^{19}	1×10^{16}	1×10^{19}	0	0
N_A (cm ⁻³)	0	0	1×10^{19}	1×10^{16}	1×10^{16}
N_t (cm ⁻³)	1×10^{15}	1×10^{15}	1×10^{14}	1×10^{14}	1×10^{14}
σ_e (cm ²)	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}
σ_h (cm ²)	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}
Defect type	Neutral	Neutral	Neutral	Single acceptor	Single acceptor

nickel (Ni) and fluorine-doped tin oxide (FTO) were 5.1 eV and 4.4 eV, respectively [18, 28]. The electron (S_e) and hole (S_h) surface recombination velocity in the FTO were kept at default setting of 1×10^5 cm/s and 1×10^7 cm/s, respectively; while that of S_e and S_h for Ni contact remained at default setting of 1×10^7 cm/s and 1×10^5 cm/s, respectively. The simulations were conducted under the standard AM1.5G illumination spectrum with an incident power density of 100 mW/cm², with a frequency of 1×10^6 Hz, a scan voltage ranging from 0 to 1.50 V, and an operating temperature of 300 K. The radiative and Auger recombination models were not activated, and their coefficients remained at the default SCAPS-1D value of zero throughout the simulations.

3. Results and discussion

3.1. Photovoltaic performance of the prototype PSCs

This section reports the photovoltaic performance of Cs₂TiBr₆ based prototype PSCs using CuO-only and CZTSe-only and CZTSe/CuO double HTLs. The intention is to select the best configuration for further improvement. Table 4 and Figure 2 compare the performance of the 3 PSCs obtained from the prototype simulations. It can be seen that the performance of the PSCs largely depends on the nature and configuration of the HTL. The CZTSe/CuO bilayer HTL-based device emerged best with the highest PCE of 12.99%. This high performance

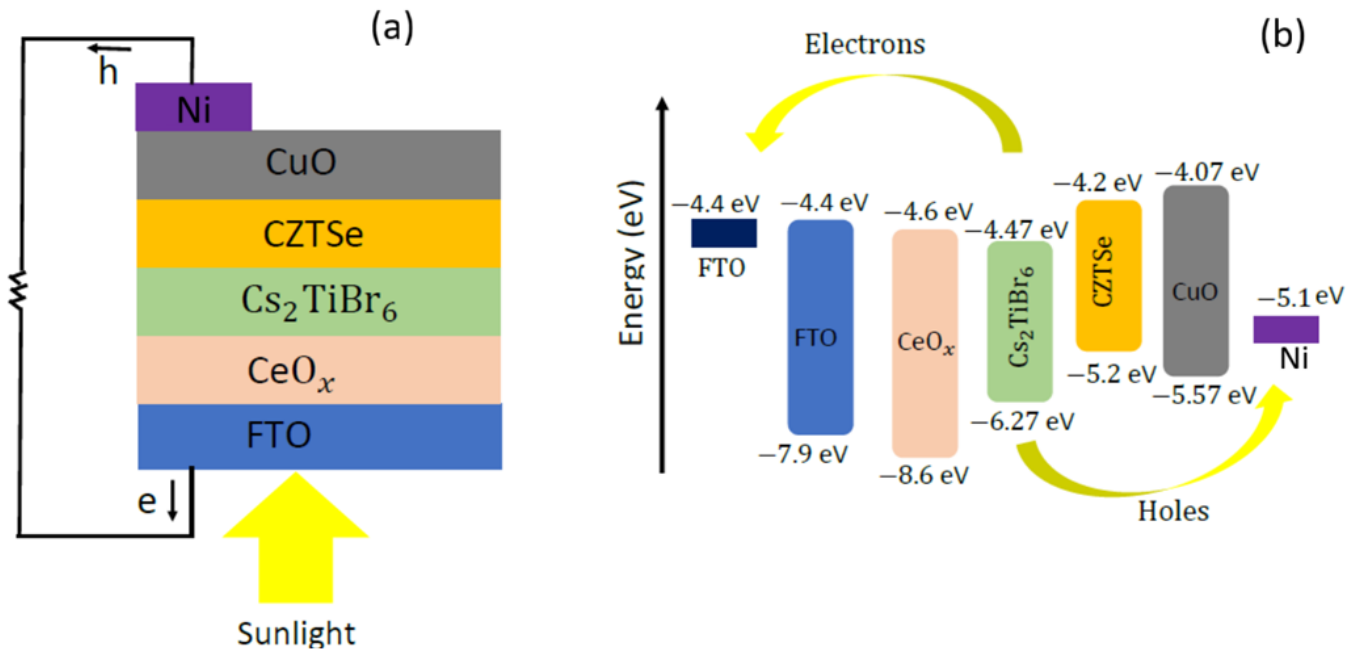


Figure 1: (a) Schematic diagram of the PSCs, (b) Energy level diagram of the various layers.

Table 2: Defect parameter employed at the various interfaces [18, 26].

Parameter	CeO _x /Cs ₂ TiBr ₆	Cs ₂ TiBr ₆ /CZTSe	CZTSe/CuO
σ_e (cm ²)	1×10^{-19}	1×10^{-19}	1×10^{-19}
σ_h (cm ²)	1×10^{-19}	1×10^{-19}	1×10^{-19}
Energetic distribution	Single	Single	Single
Defect type	Neutral	Neutral	Neutral
Energetic level with respect to E _v (eV)	0.60	0.60	0.60

Table 3: Absorption model parameters (bandgap energy, absorption edge, and coefficient A) employed in the SCAPS-1D simulation.

Layer	E_g (eV)	Absorption edge / grading first value (nm)	A coefficient constant = $A [1/(m/\sqrt{eV})]$ ($m^{-1}eV^{-\frac{1}{2}}$)	B coefficient constant ($m^{-1}eV^{-\frac{1}{2}}$)	Absorption coefficient, α (cm ⁻¹)	Model [29, 30]
FTO	3.50	354.28	5.345×10^6	0	10^4	$\alpha(h\nu) = \begin{cases} A\sqrt{h\nu - E_g}, & h\nu \geq E_g \\ 0, & h\nu < E_g \end{cases}$ where α is absorption coefficient (m ⁻¹), A is absorption coefficient parameter (m ⁻¹ eV ^{-1/2}), $h\nu$ is photon energy (eV), E_g is bandgap energy (eV).
CeO _x	3.50	354.28	5.345×10^6	0	10^4	
Cs ₂ TiBr ₆	1.80	688.88	7.454×10^6	0	10^5	
CZTSe	1.00	1239.98	1.000×10^7	0	10^5	
CuO	1.51	821.18	8.138×10^6	0	10^5	

Note:- m denotes meter.

can be attributed to synergistic improvement in charge extraction, suppressed recombination at the interface, and optimization of band alignment at the absorber/CZTSe interface.

When CuO is used as the only HTL in the configuration

(FTO/CeO_x/Cs₂TiBr₆/HTL/Ni), the device shows a moderate level of PV performance. The work function of CuO, which ranges from 5.3 to 5.5 eV aligns nicely with the valence band maximum (VBM) of Cs₂TiBr₆ at -5.2 eV, making it easier to

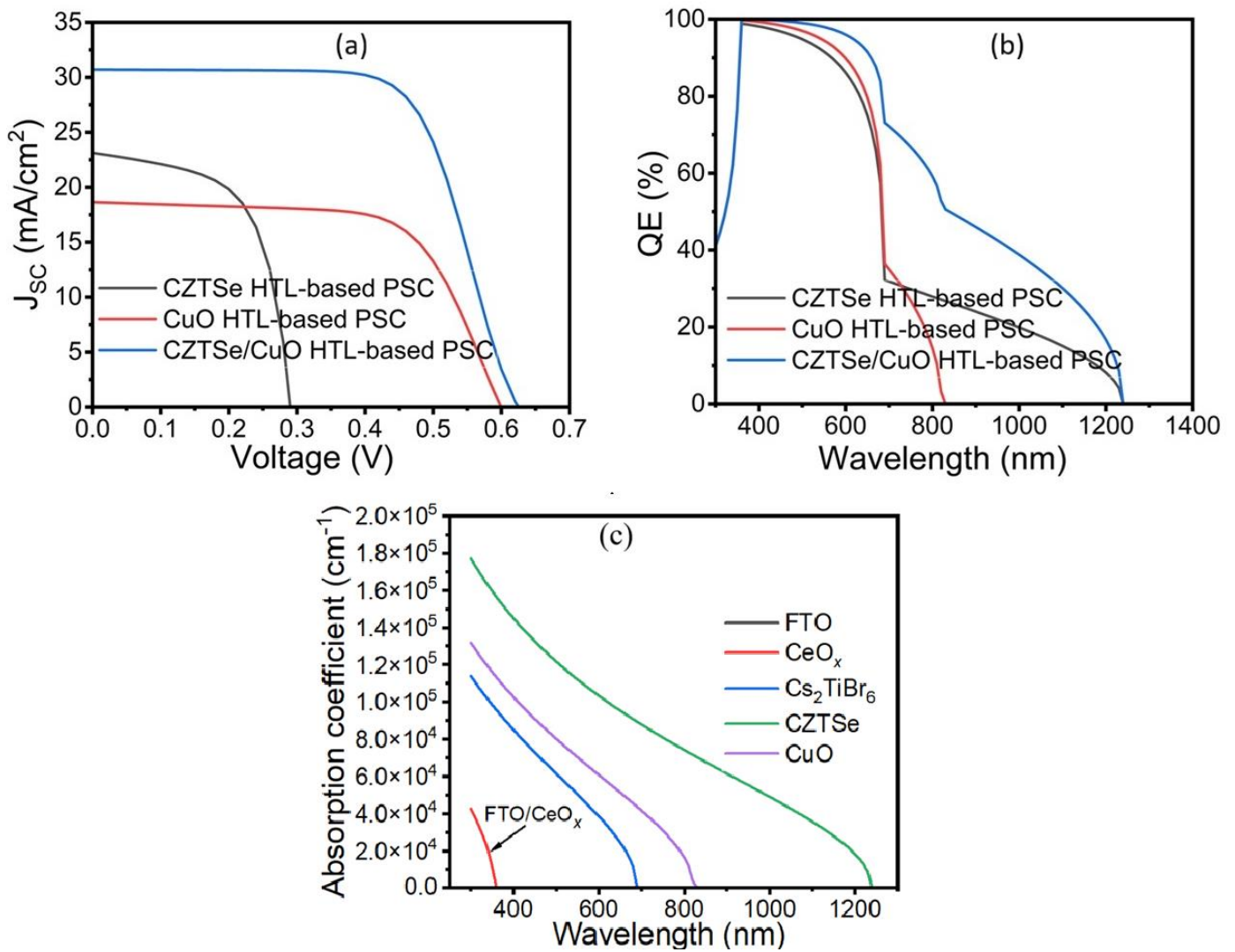


Figure 2: (a) J-V curves of the prototype PSCs, (b) Wavelength-dependent QE, (c) Optical absorption coefficient against wavelength.

Table 4: Photovoltaic performance parameters of the prototype PSCs.

Solar cell	V_{oc}	J_{sc} (mA/cm^2)	FF(%)	PCE(%)
FTO/ CeO_x / Cs_2TiBr_6 /CZTSe/Ni	0.29	23.12	60.60	4.08
FTO/ CeO_x / Cs_2TiBr_6 /CuO/Ni	0.62	18.26	60.62	6.91
FTO/ CeO_x / Cs_2TiBr_6 /CZTSe/CuO/Ni	0.62	30.70	67.74	12.99

extract holes at the Cs_2TiBr_6 /CuO interface. However, CuO's low hole mobility ($0.1 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$) and its deep defect states lead to higher series resistance and non-radiative recombination, which ultimately limits the short-circuit current density (J_{SC}) and fill factor (FF). These findings are in line with previous experimental studies on CuO-based HTLs, which emphasize its great selectivity but moderate transport capabilities [21]. The CuO-only HTL device's relatively low J_{SC} can also be attributed to its limited absorption range (300-820 nm) of the solar spectrum (Figure 2b), resulting in lower carrier generation. By contrast, the CZTSe HTL-based device (FTO/ CeO_x / Cs_2TiBr_6 /CZTSe/Ni) showed much poorer perfor-

mance metrics, suggesting better optical absorption but inadequate charge extraction. The narrow bandgap of CZTSe (1.4 eV) allows for optical absorption into the near-infrared region (up to 1235 nm), which boosts carrier generation and improves J_{SC} compared to the CuO HTL-based device. However, the lower work function (4.9-5.0 eV) and shallow VBM (~ 5.0 eV) create a less-than-ideal band offset with the Cs_2TiBr_6 absorber, leading to energy-level mismatch and interfacial recombination losses [31]. This mismatch causes a notable drop in open-circuit voltage (V_{OC}) and FF, resulting in a lower PCE.

The impressive performance of the CZTSe/CuO double HTL-based device (FTO/ CeO_x / Cs_2TiBr_6 /CZTSe/CuO/Ni)

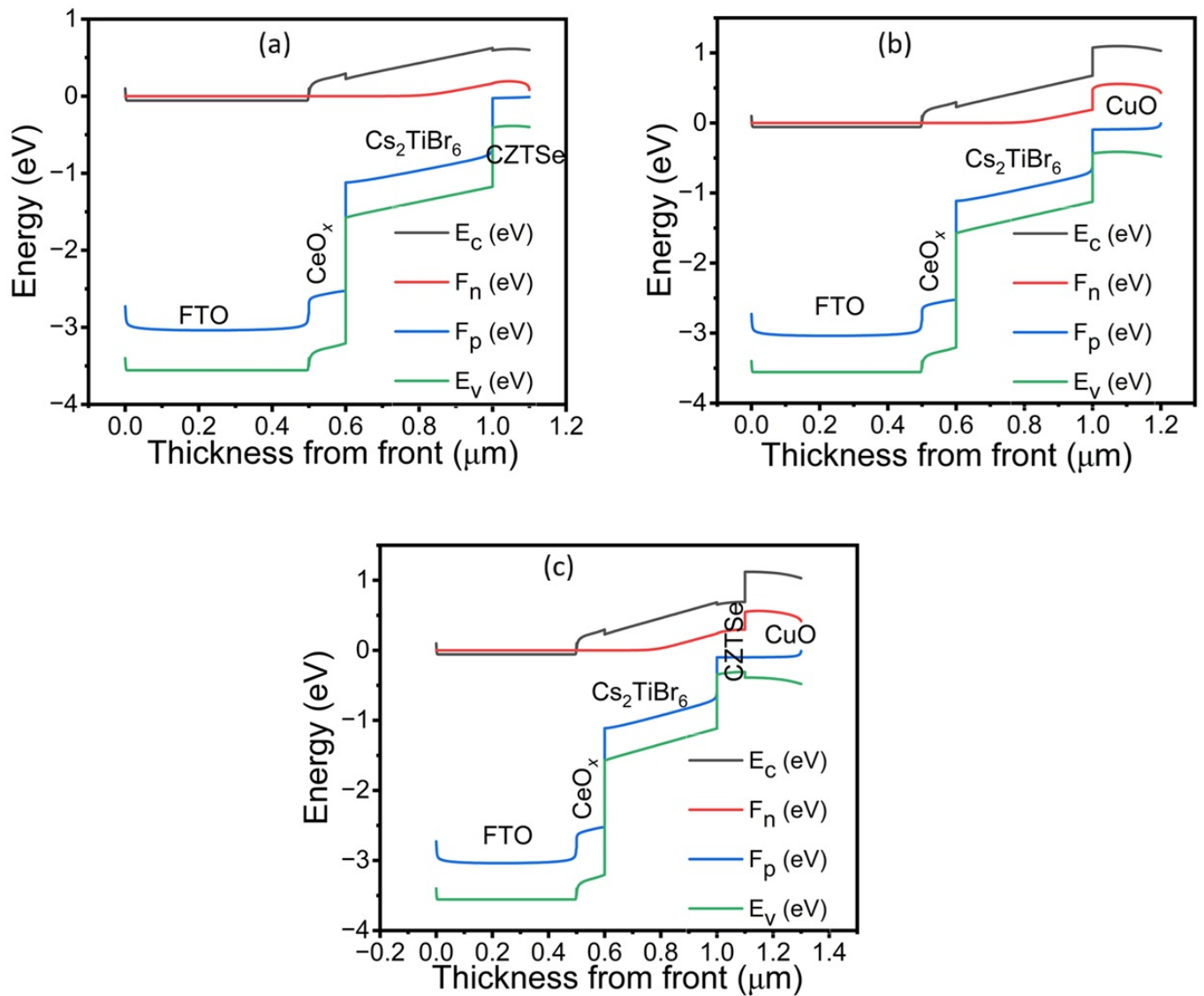


Figure 3: Energy band plots of the (a) CZTSe HTL-based PSC, (b) CuO HTL-based PSC, (c) CZTSe/CuO double HTL-based PSC.

highlights how effective it is to combine both CZTSe and CuO into a graded bilayer HTL. A significant boost in the PV parameters could be seen. The notable increases in J_{SC} and V_{OC} can be attributed to the complementary alignment of energy levels and a reduction in recombination at the rear interface. The enhanced J_{SC} is also linked to better QE and absorption in the 500–1235 nm wavelength range when compared to devices that use a single HTL. The CZTSe HTL, positioned next to the Cs₂TiBr₆ absorber, has a valence-band maximum that aligns well with that of the perovskite. This setup allows for efficient hole injection while creating a significant conduction-band offset (0.3 – 0.4 eV) that effectively prevents electron backflow. This selective transport helps reduce Shockley-Read-Hall (SRH) recombination at the Cs₂TiBr₆/CZTSe interface, which in turn enhances carrier lifetime. In addition, the higher hole mobility of CZTSe (10 cm²/V.s) makes for quicker carrier transfer

before recombination can take place. By contrast, the CuO overlayer, with its higher work function and deeper valence band maximum, acts as an energy-level bridge to the metallic Ni electrode. This creates an ohmic contact (with a hole barrier height of less than 0) and minimizes energy loss during hole collection. Additionally, the CuO HTL helps passivate surface traps at the CZTSe/Ni interface, which reduces interfacial recombination velocity and boosts the fill factor (FF). This cascading alignment (Cs₂TiBr₆/CZTSe/CuO/Ni) ensures a smooth energy gradient for hole transport while maintaining strong electron blocking to balance carrier extraction and enhance QE (Figure 2b). The moderate improvement in FF suggests that resistive and recombination losses have been effectively suppressed. Given its outstanding performance, the dual HTL device (FTO/CeO_x/Cs₂TiBr₆/CZTSe/CuO/Ni) will be further explored with varying simulation parameters to find the

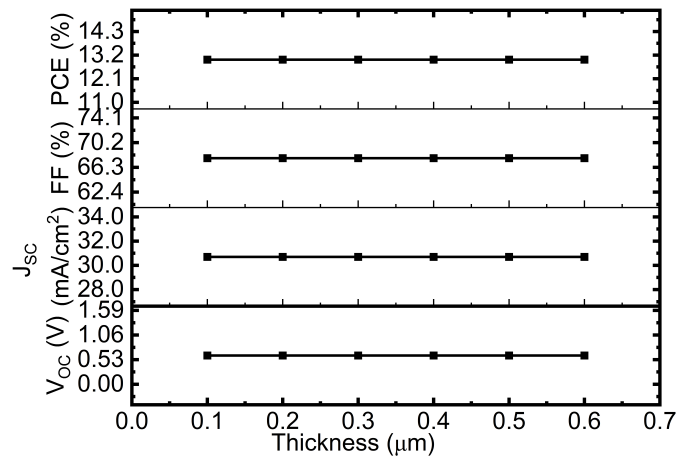


Figure 4: (a) Dependence of V_{oc} , J_{sc} , FF, and PCE on the thickness of the CeOx ETL.

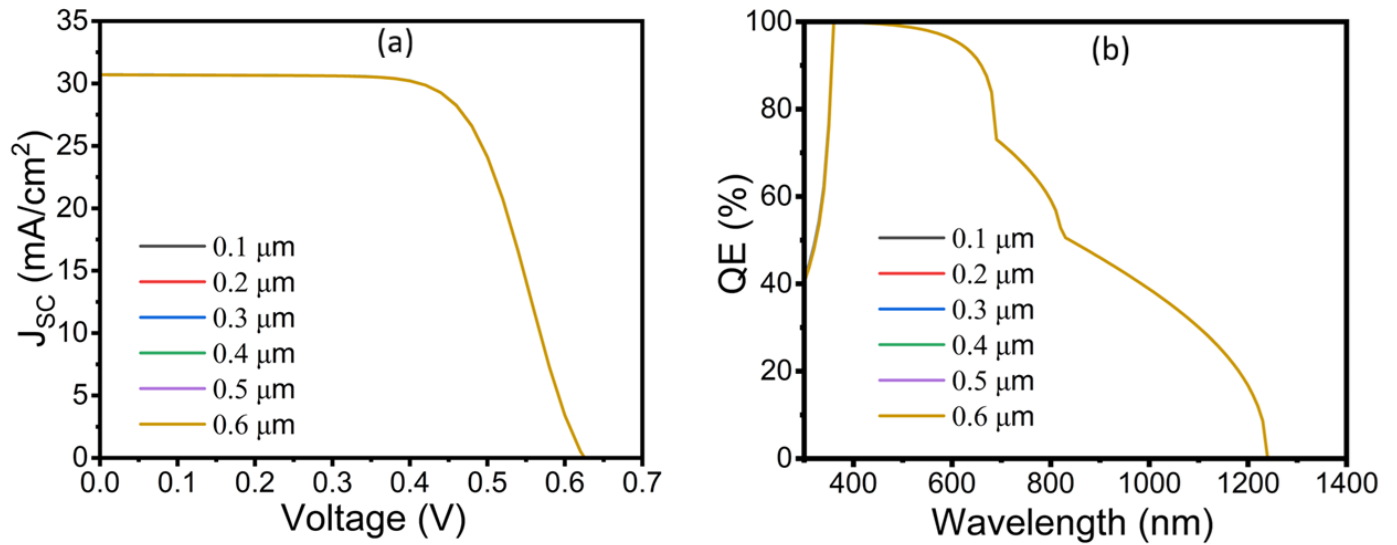


Figure 5: (a) J-V curves with varying CeOx ETL thickness, (b) QE plots.

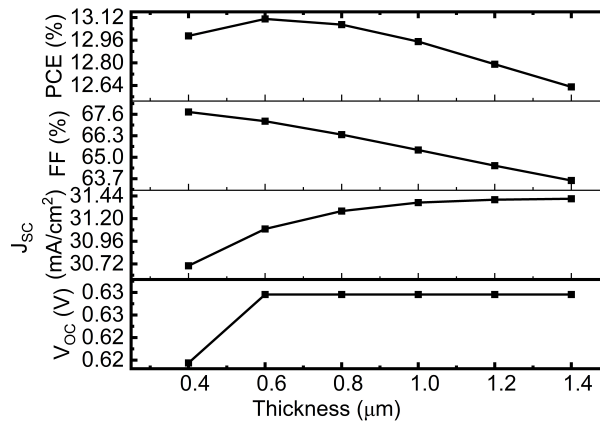


Figure 6: (a) Variation of V_{oc} , J_{sc} , FF, and PCE with thickness of absorber layer.

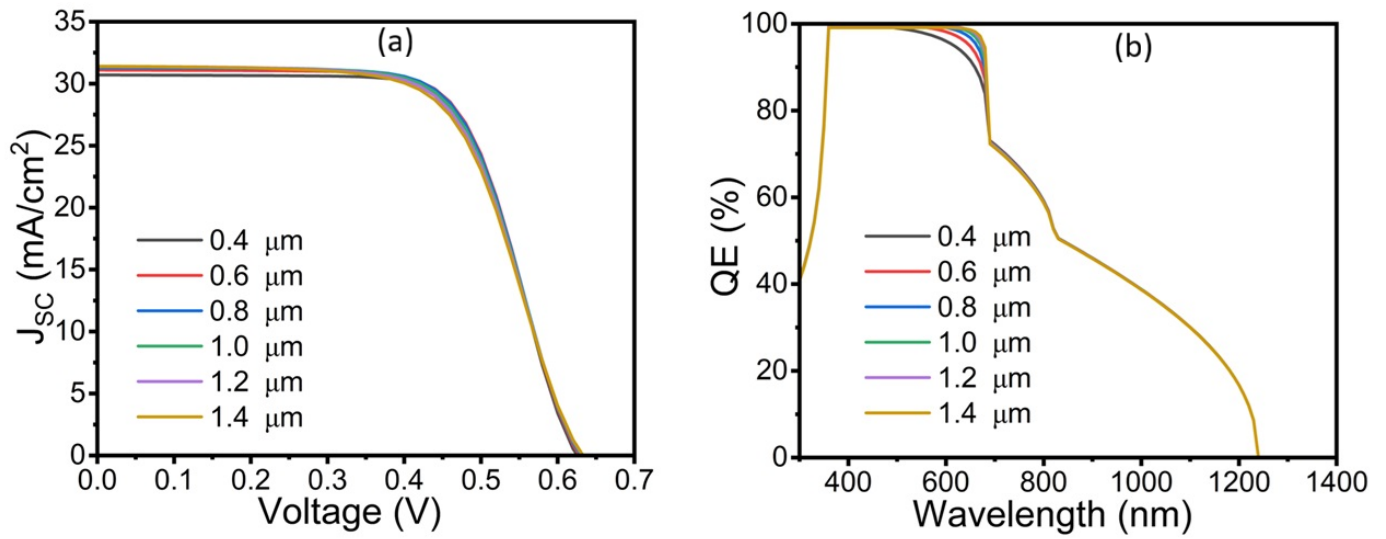


Figure 7: J-V characteristics of the device for different absorber-layer thicknesses

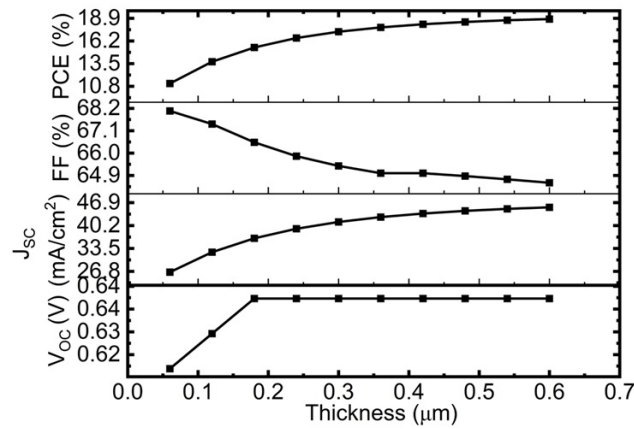
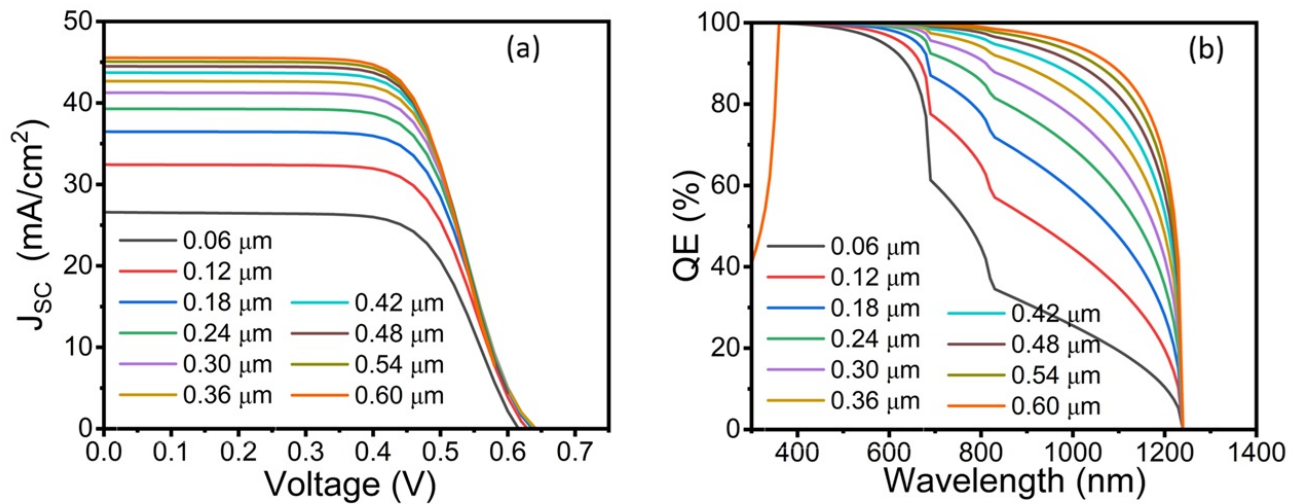
Figure 8: (a) Dependence of V_{oc} , J_{sc} , FF, and PCE on the thickness of the CZTSe HTL.

Figure 9: J-V curves with varying CZTSe HTL thickness.

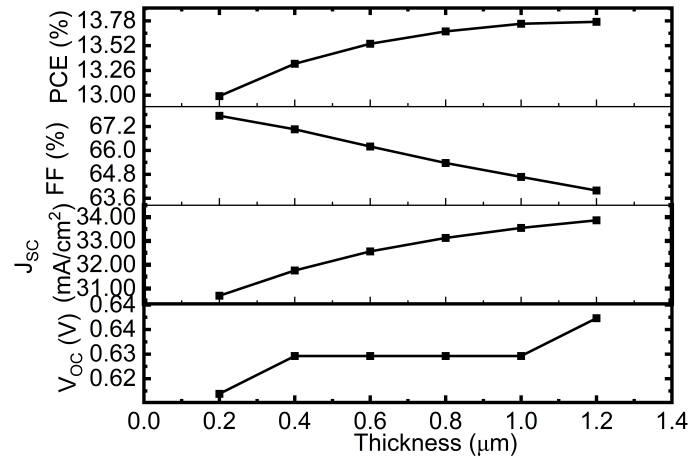


Figure 10: (a) Variation of V_{oc} , J_{sc} , FF, and PCE with thickness of CuO HTL.

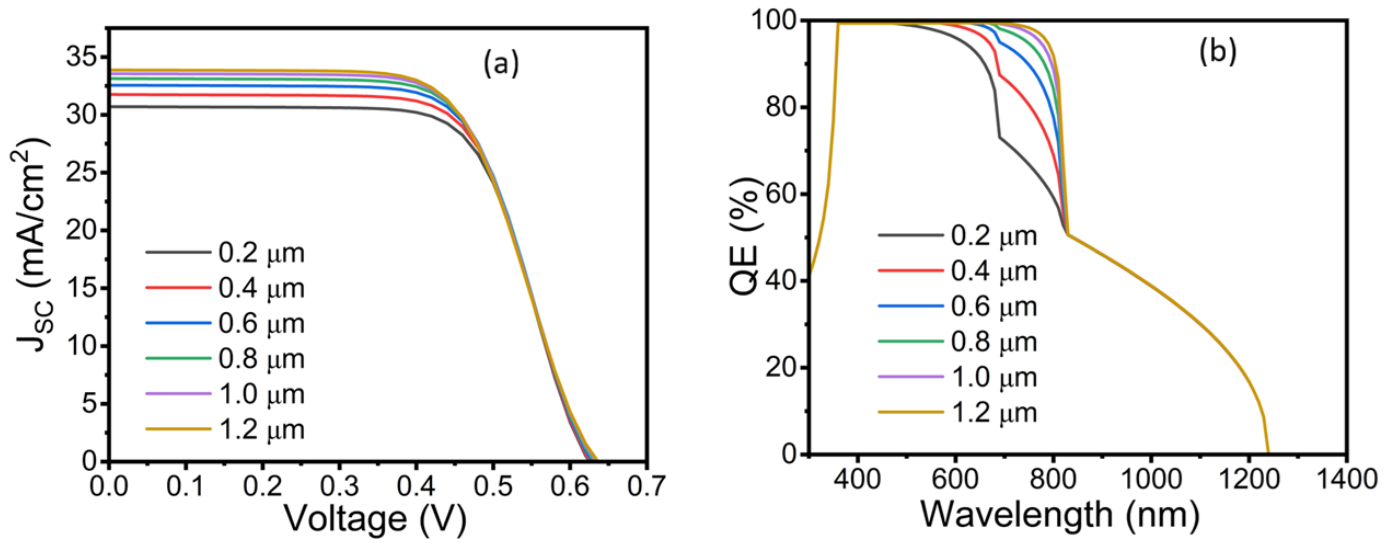


Figure 11: J-V characteristics of the device for different CuO HTL thicknesses.

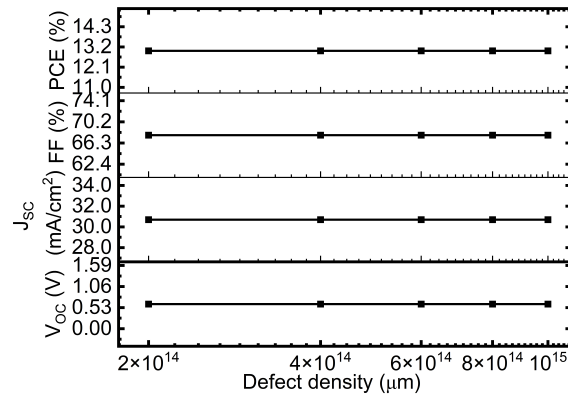


Figure 12: Variation of V_{oc} , J_{sc} , FF, and PCE with bulk defect density of CeO_x .

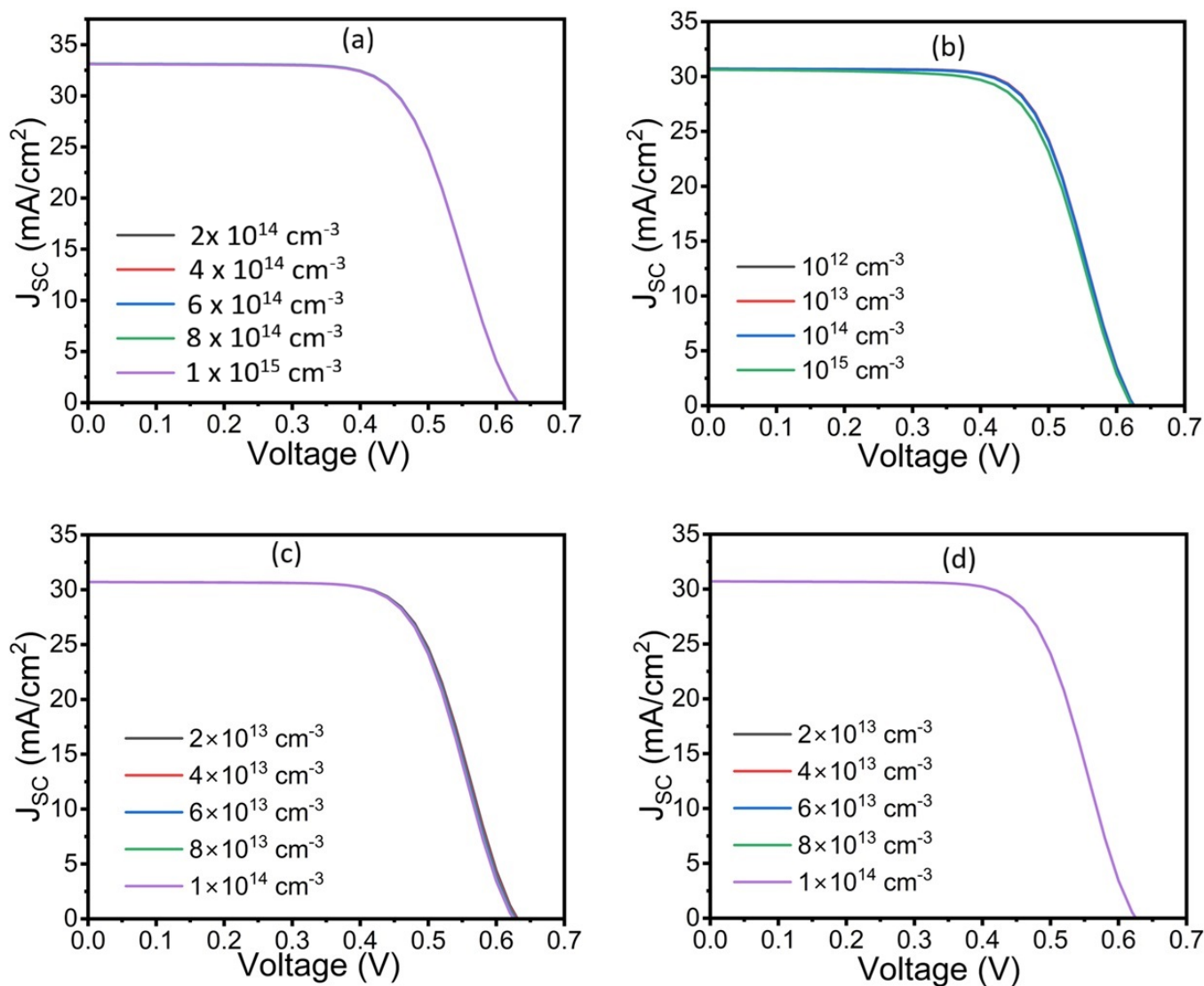


Figure 13: J-V curves with varying bulk defect density of (a) CeO_x , (b) Absorber, (c) CZTSe, (d) CuO layer.

optimal values for simulating a device with greater PCE. Meanwhile,

Figure 2c demonstrates the wavelength-dependent absorption coefficient of the constituent layers used in the device architecture. The FTO and CeO_x layers exhibit relatively low absorption coefficients and absorption edges around 354 nm, corroborating their high transparency throughout most of the visible spectrum and allowing efficient light transmission to the photoactive layers. Conversely, Cs_2TiBr_6 exhibits strong absorption within the visible region up to approximately 690 nm, consistent with its optical bandgap of 1.8 eV and its role as the primary absorber layer. Notably, CZTSe exhibits the broadest absorption range, extending to about 1240 nm due to its narrow optical bandgap (~ 1.0 eV), with a higher absorption coefficient than Cs_2TiBr_6 over a wide spectral range. This extended near-infrared optical absorption explains the enhanced QE response beyond ~ 820 nm observed in Figure 2b, proposing the interpretation of the $\text{Cs}_2\text{TiBr}_6/\text{CZTSe}$ stack as photoactive heterostruc-

ture rather than a single-absorber Cs_2TiBr_6 solar cell. Meanwhile, CuO shows intermediate absorption characteristics, extending to ~ 820 nm, contributing primarily to hole transport while providing limited additional light absorption.

Figure 3 illustrates the energy band diagrams for the 3 simulated Cs_2TiBr_6 -based PSCs. These diagrams highlight the conduction band minimum (E_C), valence band maximum (E_V), and the quasi-Fermi levels for both electrons (F_n) and holes (F_p), along with the relative band alignment across each heterojunction. Understanding these band profiles is crucial for grasping how charge separation, transport selectivity, and interfacial recombination work within the devices. For the CZTSe HTL-based device, the energy band diagram revealed that the E_C and E_V of the Cs_2TiBr_6 absorber were -4.47 eV and -6.27 eV, respectively. The CeO_x ETL has an E_C of -4.4 eV, which aligns nicely with Cs_2TiBr_6 , ensuring efficient electron injection from the absorber to the FTO electrode. By contrast, the CZTSe HTL shows an E_V of -5.5 eV and an E_C of -4.5 eV. This

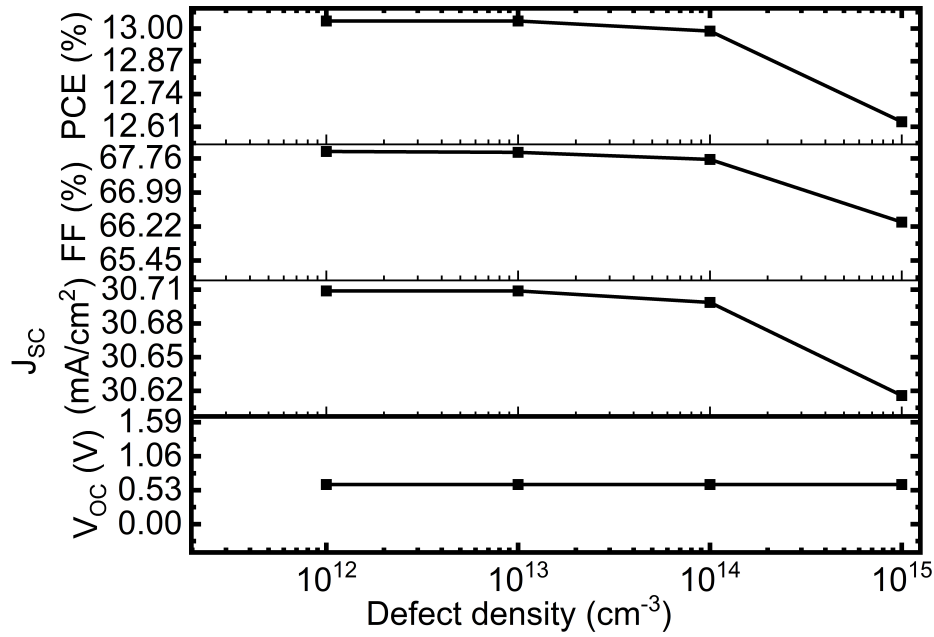


Figure 14: Dependence of V_{oc} , J_{sc} , FF, and PCE with bulk defect density of absorber layer.

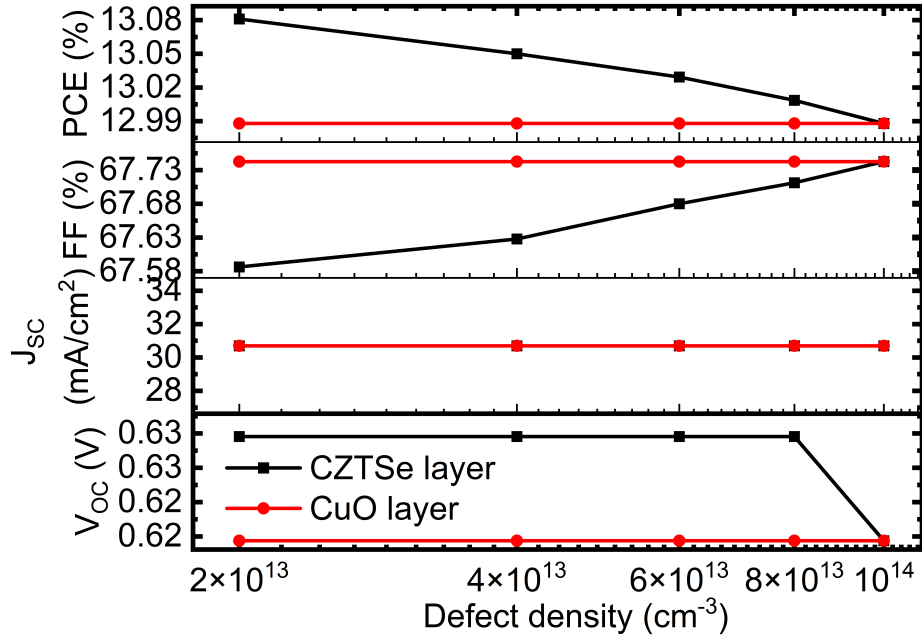


Figure 15: Variation of V_{oc} , J_{sc} , FF, and PCE with defect density of the CZTSe and CuO layer.

stack results in a valence band offset (ΔE_V) of about 0.77 eV at the $\text{Cs}_2\text{TiBr}_6/\text{CZTSe}$ interface, creating an energy barrier that hinders hole extraction. Meanwhile, a small conduction band offset (ΔE_C) of 0.03 eV can lead to unwanted electron leakage into the HTL to promote interfacial recombination. This combination resulted in poor carrier selectivity, which explains the low V_{oc} (0.29 V) and the lower PCE (4.08%) observed for this structure. Additionally, the steep band bending near the

$\text{Cs}_2\text{TiBr}_6/\text{CZTSe}$ junction further indicated charge accumulation and non-radiative losses at this interface.

Figure 3b shows the energy band diagram for the CuO-based device. CuO has a EV of -5.58 eV, which results in a smaller ΔE_V of 0.69 eV compared to the Cs_2TiBr_6 absorber. This adjustment helps improve hole extraction when compared to the device that only uses CZTSe. Additionally, the E_C of CuO (-4.07 eV) is significantly lower than that of Cs_2TiBr_6 ,

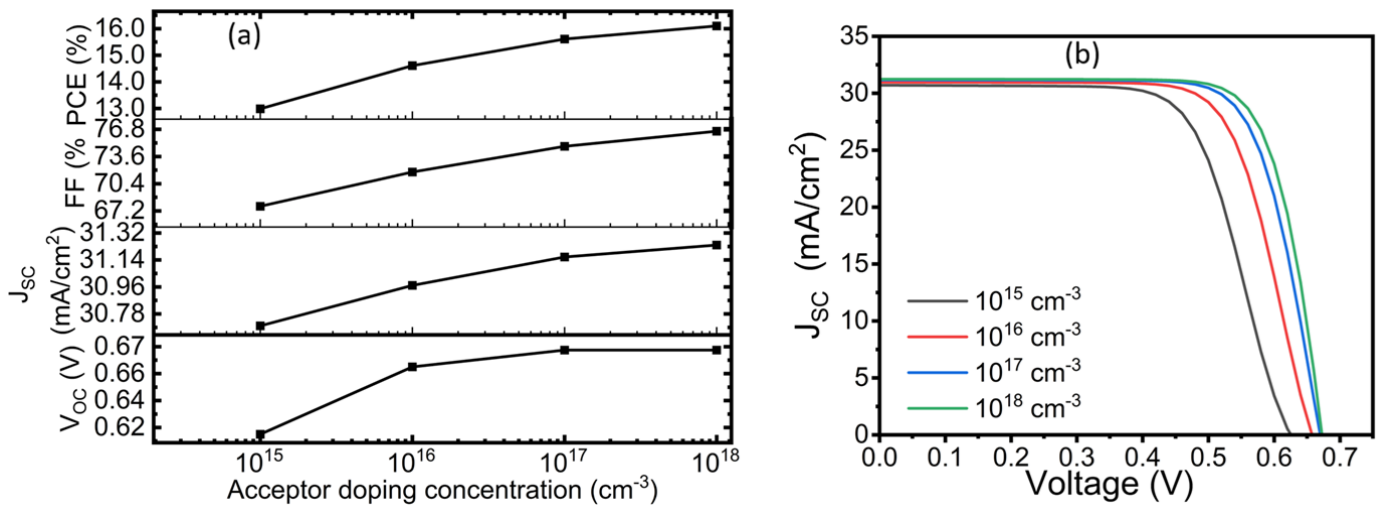


Figure 16: (a) Dependence of V_{oc} , J_{sc} , FF, and PCE with acceptor doping concentration of CuO layer, (b) Corresponding J-V curves.

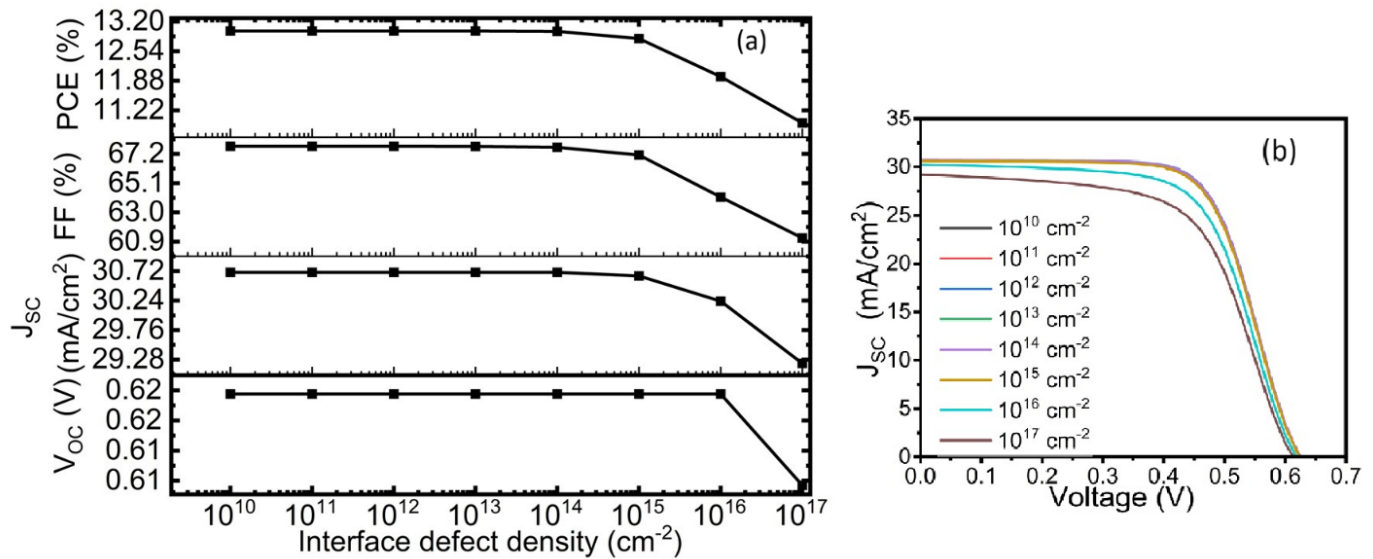


Figure 17: Variation of V_{oc} , J_{sc} , FF, and PCE with defect density of CeOx/Cs₂TiBr₆ interface, (b) J-V curves.

creating a larger electron-blocking barrier of 0.4 eV. This effectively prevents electron backflow into the HTL. Thanks to this favorable band alignment, the CuO layer enhances charge selectivity, leading to better charge separation and fewer interfacial recombination losses. Consequently, the CuO HTL-based PSC shows a much higher V_{oc} and FF compared to the CZTSe HTL-based device. However, as stated earlier, CuO's relatively low hole mobility limits charge transfer, resulting in a moderate J_{sc} and capping the PCE at 6.91%. This PSC also displays smoother band transitions than the CZTSe-based cell, but some band bending near the CuO/Ni interface suggests resistive losses and a partial barrier for holes. This is due to a slight misalignment in the Fermi levels between the work functions of CuO (5.3 eV) and Ni (5.1 eV).

The double HTL configuration (Figure 3c) exhibits an op-

timized stepwise energy alignment that substantially improves carrier extraction. The addition of a CZTSe HTL interlayer between Cs₂TiBr₆ and CuO provides an intermediate E_v position (−5.5 eV for CZTSe vs. −5.58 eV for CuO) to form a sequential energy gradient for hole transport from the absorber to the back electrode. This gradual alignment reduced interfacial potential barriers to minimize hole reflection, and to ensure smoother carrier flow across the interfaces. Simultaneously, the E_c of CZTSe (−4.5 eV) lies below that of Cs₂TiBr₆ (−4.47 eV) to form a small E_c offset (0.03 eV) that effectively confined photogenerated electrons within the absorber and prevented recombination at the HTL side. The integration of CuO overlayer contributes to form an ohmic contact with the Ni electrode and improved Fermi-level matching (because both possess high work functions ~5.0 eV). The resulting band structure produced

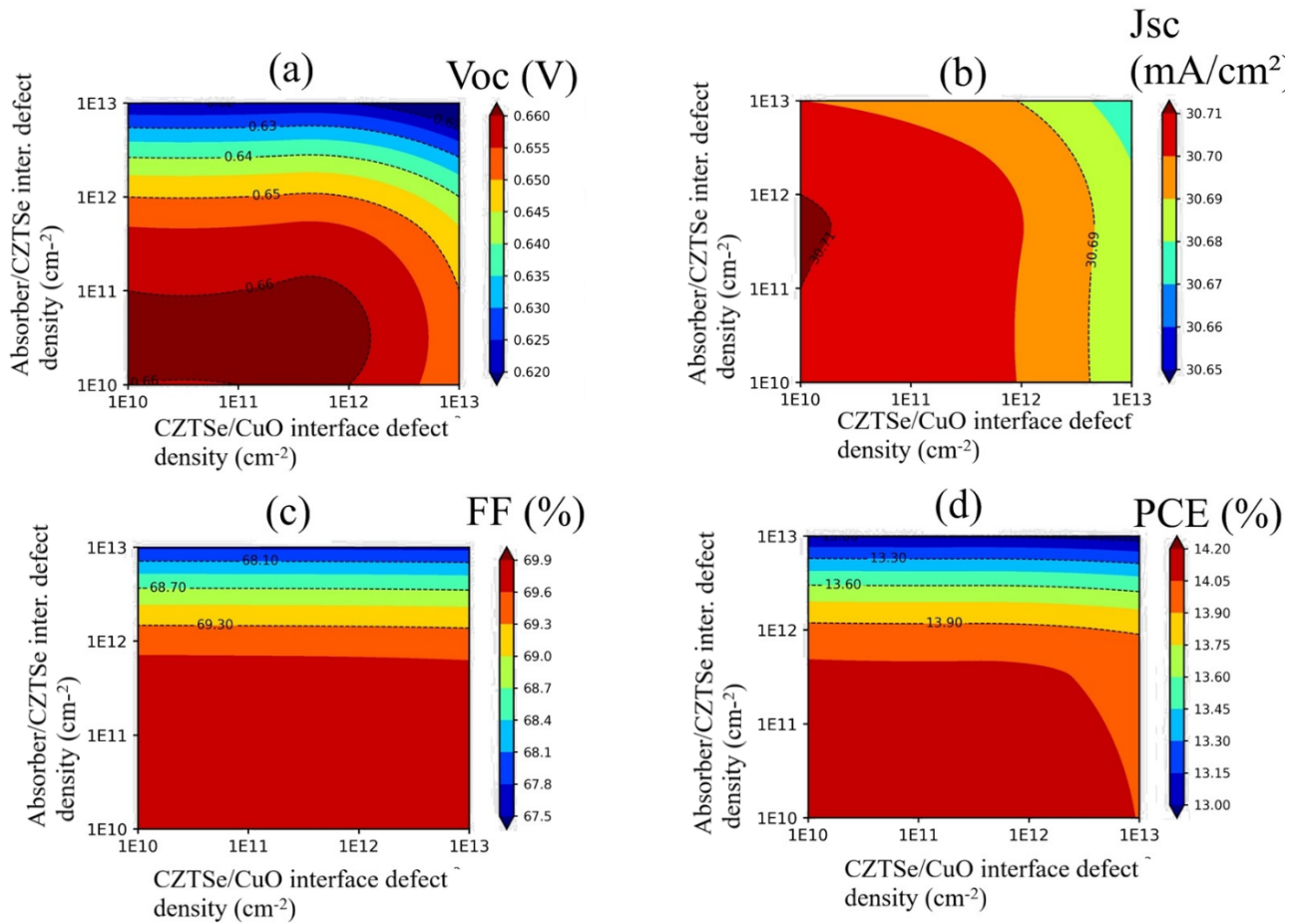


Figure 18: Contour mapping for varying (a) V_{oc} , (b) J_{sc} , (c) FF, and (d) PCE on the defect densities of the absorber/CZTSe and CZTSe/CuO interfaces.

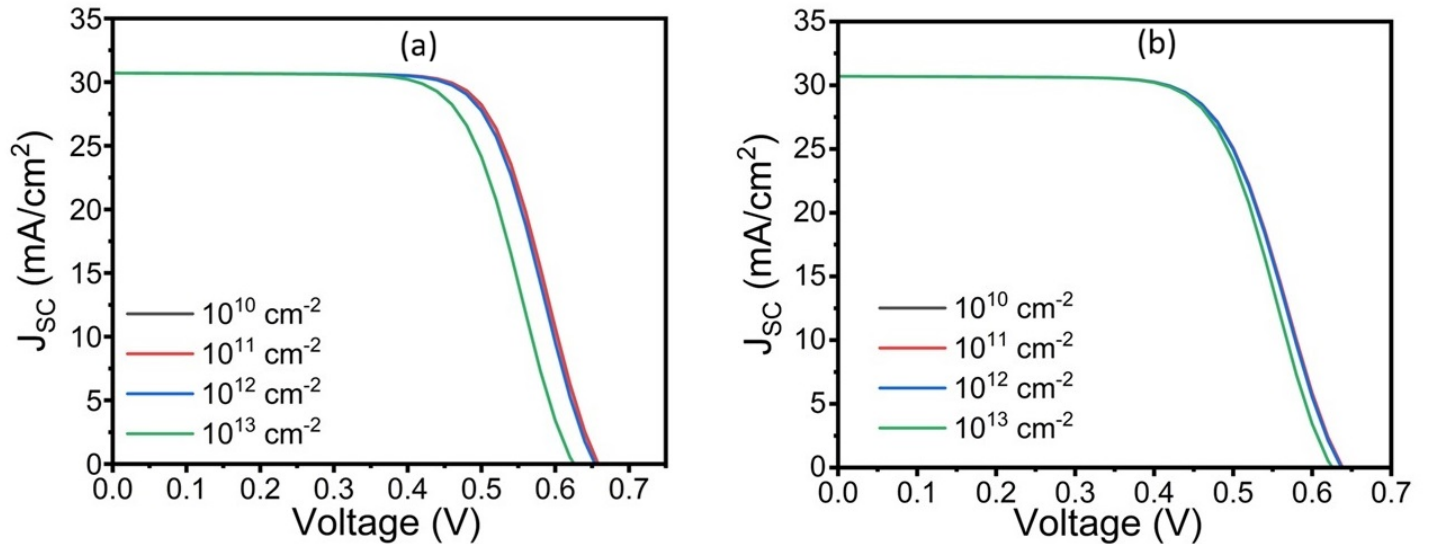


Figure 19: J-V characteristics with varying interface defect density of (a) Cs₂TiBr₆/CZTSe, (b) CZTSe/CuO.

a built-in electric field across the perovskite and HTL layers to enhance both carrier separation and drift transport. This opti-

mized band arrangement supports the improvement in PV performance of the CZTSe/CuO double HTL-based device.

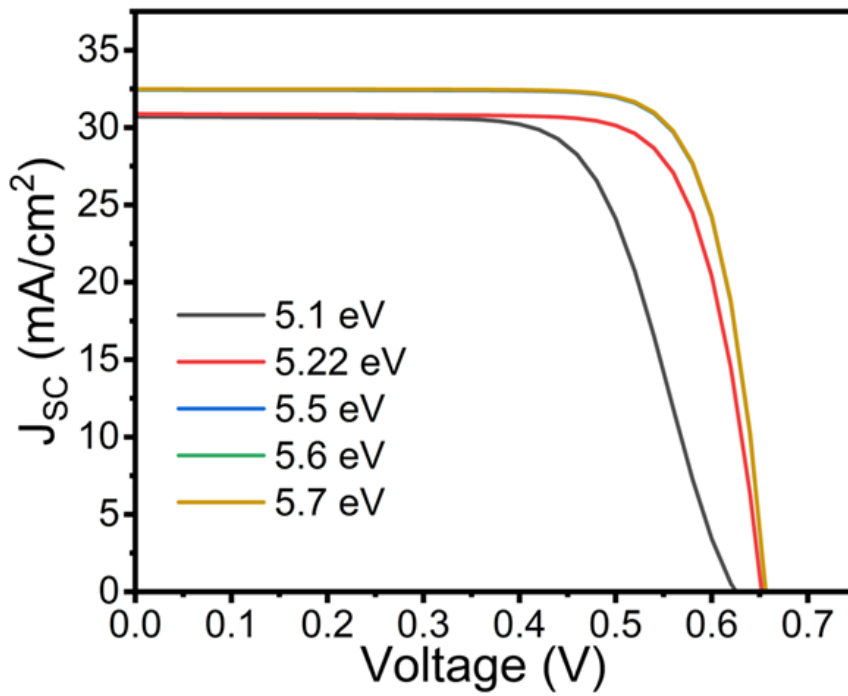


Figure 20: J-V characteristics with varying work function of the back metal.

3.2. Influence of thickness of the CeO_x ETL layer

This section looks into how changing the thickness (0.1 – 0.6 μm) of the CeO_x layer affects the PV performance of the FTO/ CeO_x / Cs_2TiBr_6 /CZTSe/CuO/Ni PSC. The key performance metrics remain constant, where V_{OC} , J_{SC} , FF and PCE stay at 0.62 V, 30.70 mA/cm^2 , 67.74%, and 12.99%, respectively (Figures 4 and 5). This consistent performance can be linked to the excellent band alignment and high conductivity at the CeO_x / Cs_2TiBr_6 interface. The E_{C} of CeO_x aligns nicely with that of Cs_2TiBr_6 , resulting in a minimal ΔE_{C} of 0.07 eV. This alignment facilitates efficient electron extraction and transport from the Cs_2TiBr_6 absorber to the front FTO contact, while still providing a sufficient barrier for holes, thanks to the large bandgap (3.5 eV) of CeO_x . A similar observation was made by Dong *et al.* [32] regarding low-temperature processed CeO_x ETL in PSCs.

The wide optical bandgap of CeO_x provides minimal parasitic absorption within the visible region, so that an increase in thickness (0.1 – 0.6 μm) does not introduce significant optical losses. Therefore, generation rate of photocarriers in Cs_2TiBr_6 remained unaffected, keeping the value of J_{SC} unchanged. This result agrees with the overlapping QE curves (Figure 5b), suggesting there is no change in photon absorption. Additionally, the high electron mobility (100 $\text{cm}^2/\text{V.s}$) and moderate donor doping concentration (10^{16} cm^{-3}) renders the layer highly conductive. Therefore, series resistance remained negligible to maintain constant value of FF and PCE.

In n-i-p junction PSCs, the electric field and built-in potential mainly develop at the ETL/absorber interface. So, once the CeO_x ETL creates a solid, pinhole-free film, adding more thickness does not really change the interfacial recombination

dynamics. The steady V_{OC} and FF values indicate that the losses from recombination are not influenced by the thickness of the ETL. Moiz *et al.* (2022) [33] and Karmaker *et al.* (2023) [12] reached similar findings for Cs_2TiBr_6 -based PSCs, showing that factors like defect passivation and interface energetics play a significant role in performance than geometric aspects. In real-world applications, very thin CeO_x layers (<80 nm) might face issues like incomplete coverage and shunting, while thicker layers (>600 nm) could compromise transparency or create mechanical stress during production. Therefore, it's crucial to find a CeO_x thickness that strikes the right balance between optical transparency, electrical conductivity, and interfacial stability to ensure efficient electron transport in lead-free Cs_2TiBr_6 PSCs.

3.3. Influence of thickness of the absorber layer

The absorber layer plays a crucial role in determining the performance of PSCs, as it controls both light absorption and carrier transport. Figures 6 and 7 shows the effect of varying the thickness of the Cs_2TiBr_6 absorber (0.4–1.4 μm) on the performance of the FTO/ CeO_x / Cs_2TiBr_6 /CZTSe/CuO/Ni device. The V_{OC} (0.62 – 0.63 V) and J_{SC} (30.70 – 31.41 mA/cm^2) exhibits slight increases with an increase in absorber thickness. However, the FF (67.74 – 63.59%) gradually declined, resulting to an optimal PCE of 13.11% at a Cs_2TiBr_6 thickness of 0.6 μm , followed by a gradual decline beyond this point. The improved J_{SC} (30.70 – 31.41 mA/cm^2) with absorber thickness can be attributed to boosted photon absorption, as can be seen in the improved QE in the wavelength range 510–620 nm (Figure 7b). The indirect bandgap of Cs_2TiBr_6 (1.8 eV) enables efficient optical absorption in the visible spectrum up to ~700 nm. How-

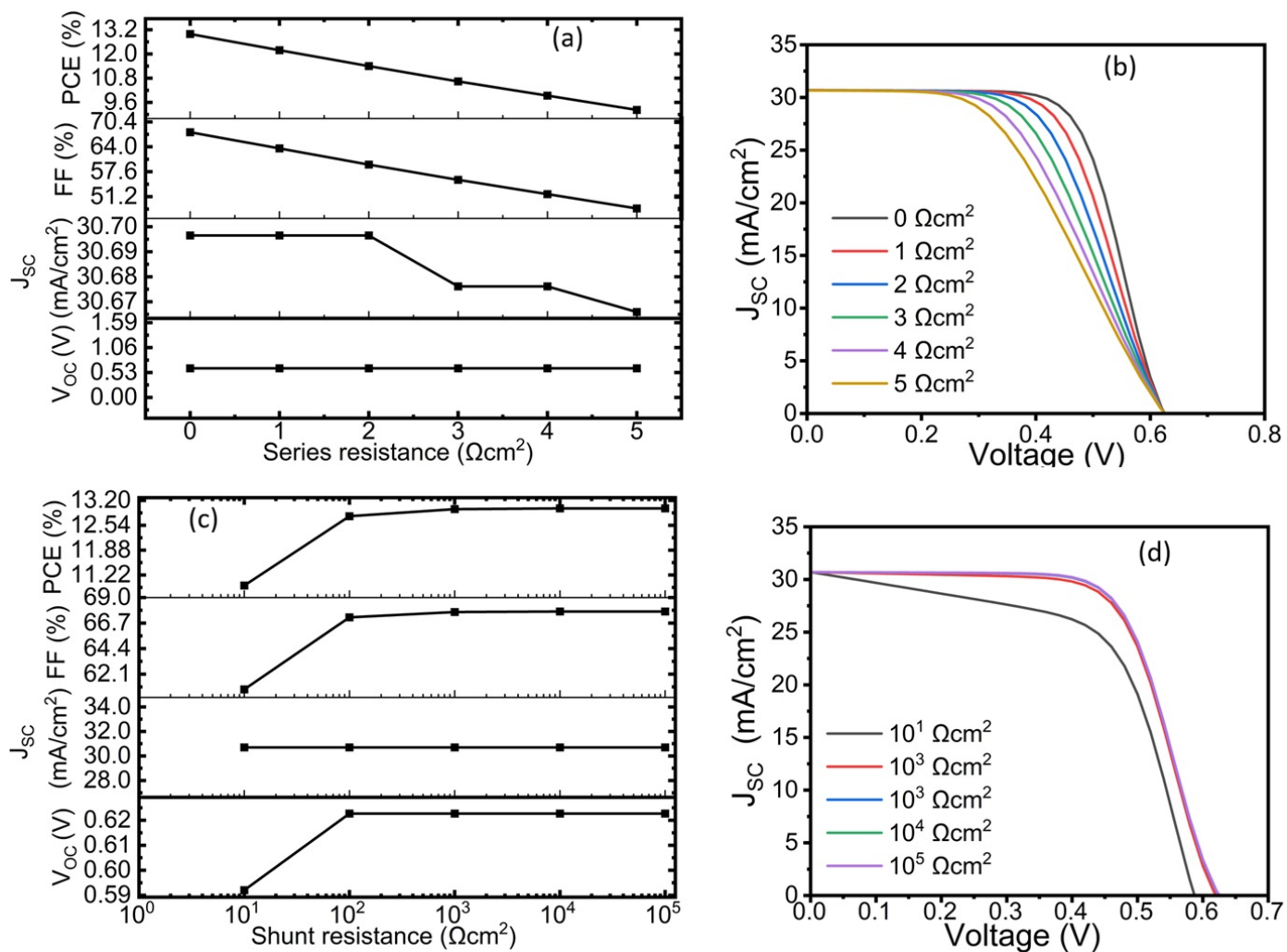


Figure 21: (a) Changes in values of V_{oc} , J_{sc} , FF, and PCE with series resistance, (b) J-V curves for the varied series resistance, (c) Dependence of V_{oc} , J_{sc} , FF, and PCE on shunt resistance, (d) J-V curves for the varied shunt resistance.

ever, its relatively low absorption coefficient ($10^4 - 10^5 \text{ cm}^{-1}$) compared to lead halide perovskites ($10^5 - 10^6 \text{ cm}^{-1}$) suggest that thicker layers are required to absorb a greater portion of incident photons. Therefore, an increase in thickness ($0.4 - 1.0 \mu\text{m}$) results in more photogenerated carriers due to increased light absorption, which increased J_{sc} . However, an increase in thickness beyond $1.0 \mu\text{m}$, produced a marginal increase in J_{sc} due to optical absorption saturation, as most above-bandgap photons were already captured within the front portion of the absorber layer. A similar thickness-dependent behavior has been reported for a simulation work on Cs_2TiBr_6 , where the J_{sc} tends to saturate beyond $0.8 \mu\text{m}$ due to the limited optical absorption coefficient [12].

The nearly constant V_{oc} ($0.62 - 0.63 \text{ V}$) across the varied thickness indicates that recombination dynamics within the absorber remains unchanged. Usually, V_{oc} is controlled by the quasi-Fermi level separation, which is determined by the balance between carrier photogeneration and recombination [34]. In contrast, the gradual decrease exhibited by the FF can be at-

tributed to the increased carrier transport distance and series resistance as the absorber thickness increases. When the absorber thickness exceeds the carrier diffusion length, photogenerated carriers deep within the absorber experience higher recombination losses before reaching the contact. The balance between enhanced absorption and increased recombination explained the peak PCE at $0.6 \mu\text{m}$, beyond which PCE declines despite slightly higher J_{sc} . This trade-off between optical enhancement and transport losses is a common feature in PSCs and has been extensively studied by numerical simulations, where an absorber thickness of $0.6 - 0.8 \mu\text{m}$ often yields the best compromise between J_{sc} , V_{oc} , and FF [12, 34]. Further improvement in performance at higher thicknesses can be achieved by adopting strategies such as, (i) boosting carrier mobilities through compositional tuning or defect passivation; (ii) reducing defect densities via low-temperature crystallization or halide additive engineering; (iii) incorporating back/ rear reflectors or textured interfaces to increase the optical path length without increasing physical thickness; and (iv) enhancing energy-band alignment

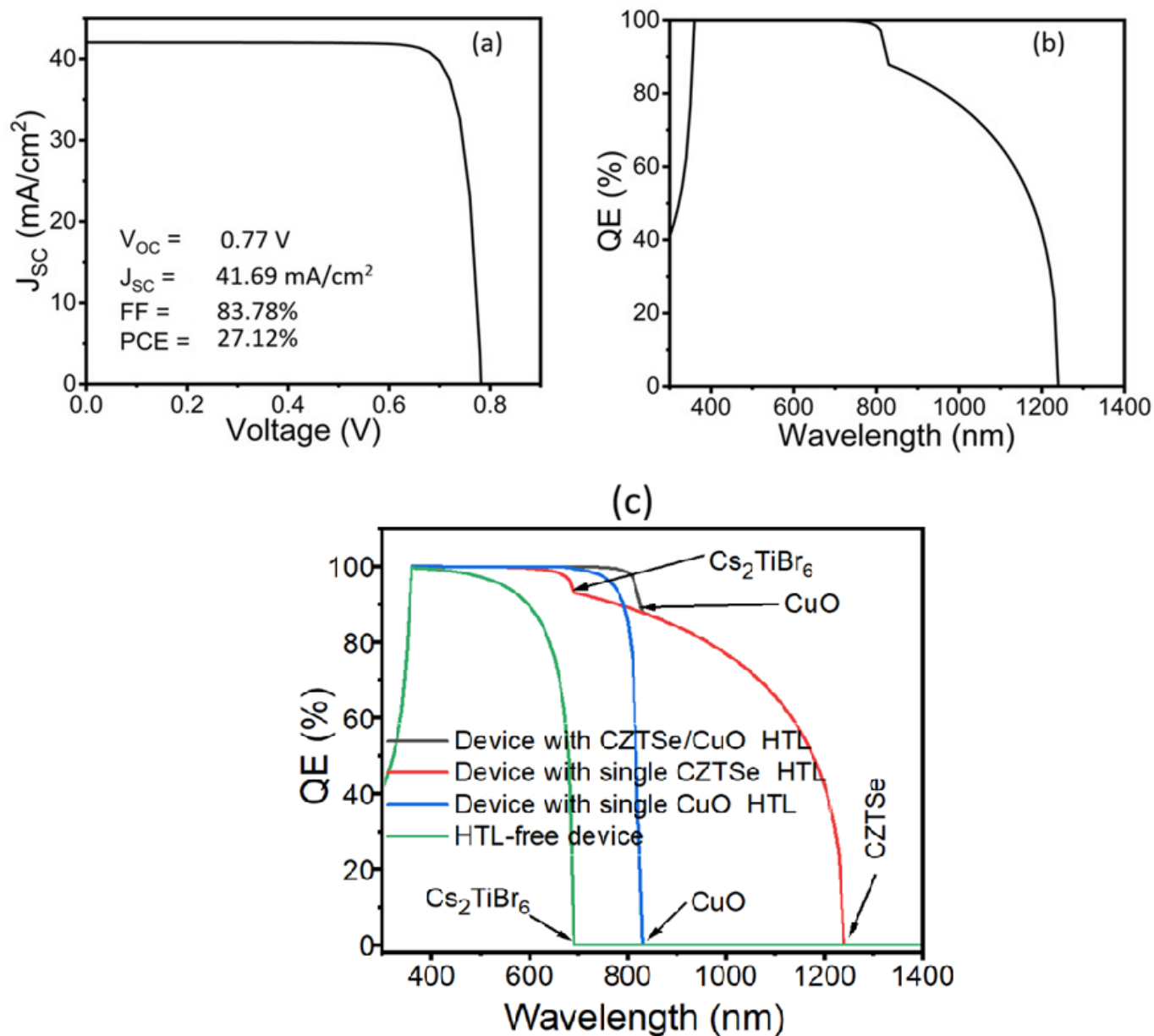


Figure 22: (a) J-V curve for the optimized CZTSe/CuO double HTL-based PSC, (b) QE curve, (c) QEs of the optimized devices utilizing CZTSe/CuO double HTL, CZTSe single HTL, CuO single HTL, HTL-free configuration.

between the absorber and the CZTSe/CuO hole transport layers to reduce interfacial recombination.

3.4. Influence of CZTSe HTL thickness

Figures 8, 9 illustrates the effect of CZTSe HTL thickness on PV parameters in the thickness range 0.06 – 0.60 μ m. The CZTSe acts as the first HTL situated between the absorber and the second stacked CuO HTL. Unlike the absorber layer, where thickness mainly dictates how well it absorbs light, the thickness of CZTSe plays a crucial role in the device's performance by affecting carrier transport dynamics, recombination behavior, interfacial selectivity, and resistive effects. A variation in the thickness of CZTSe (0.06 – 0.60 μ m) produce a consistent

boost in J_{SC} and PCE, though a slight leveling off of V_{OC} and a gradual decline in the FF are observed.

At very small thicknesses (0.06 and 0.12 μ m), the HTL is too small to fully establish efficient hole selectivity at the Cs_2TiBr_6 /CZTSe interface. In this regime, the thin CZTSe layer provides limited spatial separation between the absorber and back contact, which allow partial electron leakage toward the rear electrode. Such leakage increases interfacial recombination and reduces effective carrier extraction efficiency. Furthermore, insufficient HTL thickness may not adequately screen interface defect states at the Cs_2TiBr_6 /CZTSe interface, leading to increased Shockley-Read-Hall (SRH) recombination. As a result, both J_{SC} and V_{OC} tend to be lower at these small

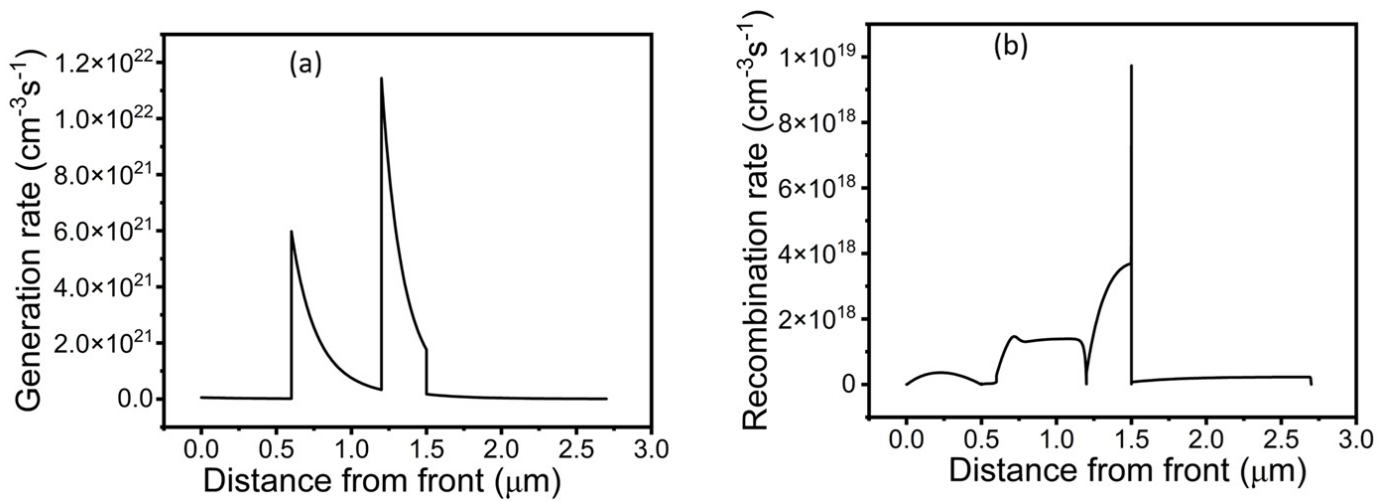


Figure 23: (a) Carrier generation rate for the ETL-assisted cell, (b) Carrier recombination rate for the ETL-assisted cell.

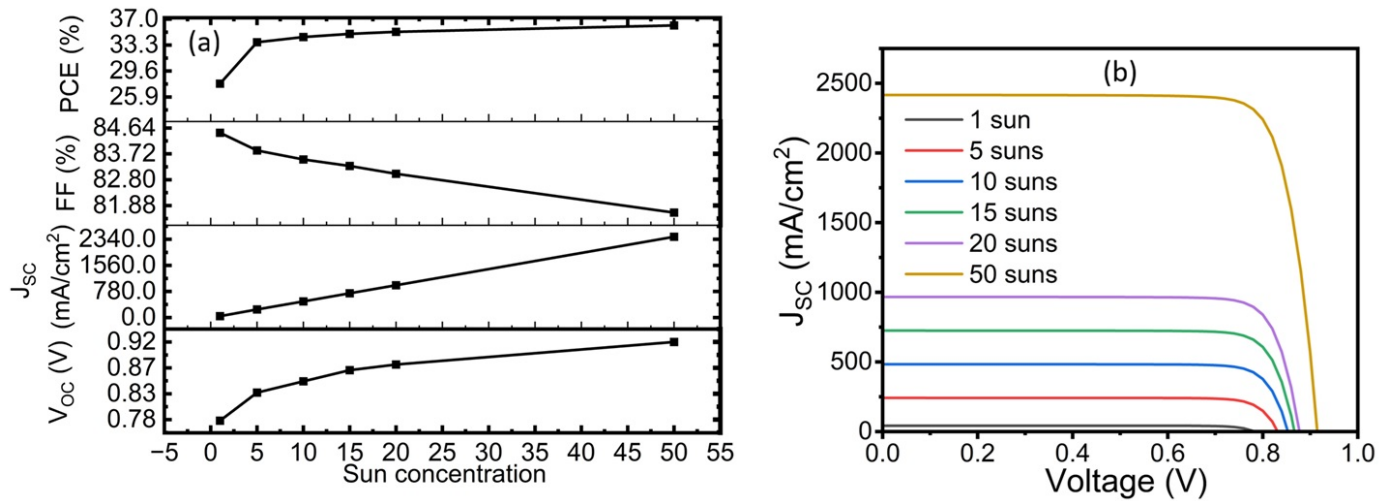


Figure 24: Dependence of V_{oc} , J_{sc} , FF and PCE on sun concentration, (b) J-V curves.

thicknesses, causing the device to operate in a transport-limited regime.

An increase in thickness (0.18–0.36 μm) leads to a significant improvement in device performance. The HTL becomes reasonably thick to provide effective hole selectivity and suppress electron back-injection from the absorber toward the rear contact. The increased thickness enhances the electron-blocking capability of the CZTSe layer by increasing the barrier width, thereby reducing interfacial recombination. Simultaneously, improved hole extraction reduces carrier accumulation at the $\text{Cs}_2\text{TiBr}_6/\text{CZTSe}$ interface, resulting in enhanced quasi-Fermi level splitting. This explains the slight increase in V_{oc} (0.62–0.64 V) and the substantial increase in J_{sc} (36.47–42.68 mA/cm^2). The improvement in J_{sc} is ascribed to improved carrier collection efficiency and reduced recombination losses at the back interface. It can also be traced to an improvement in QE between 650–1200 nm wavelength (Figure 9b), suggesting improved photon absorption and carrier generation. Beyond

thickness of 0.42 μm , the device enters a regime where further increases in thickness yield gradual improvements, where the values of J_{sc} , FF and PCE increase as 43.72–45.54 mA/cm^2 , 65.01–64.54%, and 18.19–18.81%, respectively. Although the inhibition of interfacial recombination continues to be effective, the augmented thickness leads to an increase in bulk transport resistance within the HTL. As the thickness increases, the distance that holes must travel becomes longer, leading to a higher resistive voltage drop when under forward bias. This is observed as a gradual decrease in the FF (68.07–64.54%). Furthermore, because recombination is proportional to volume, the SRH recombination within the HTL experiences a slight increase with thickness, which further exacerbates the degradation of the FF.

The V_{oc} exhibits saturation behavior beyond 0.18 μm . According to [34], where J_0 is the saturation current density, V_{oc} depends logarithmically on the ratio of photogenerated current to recombination current. Although J_{sc} continues to increase

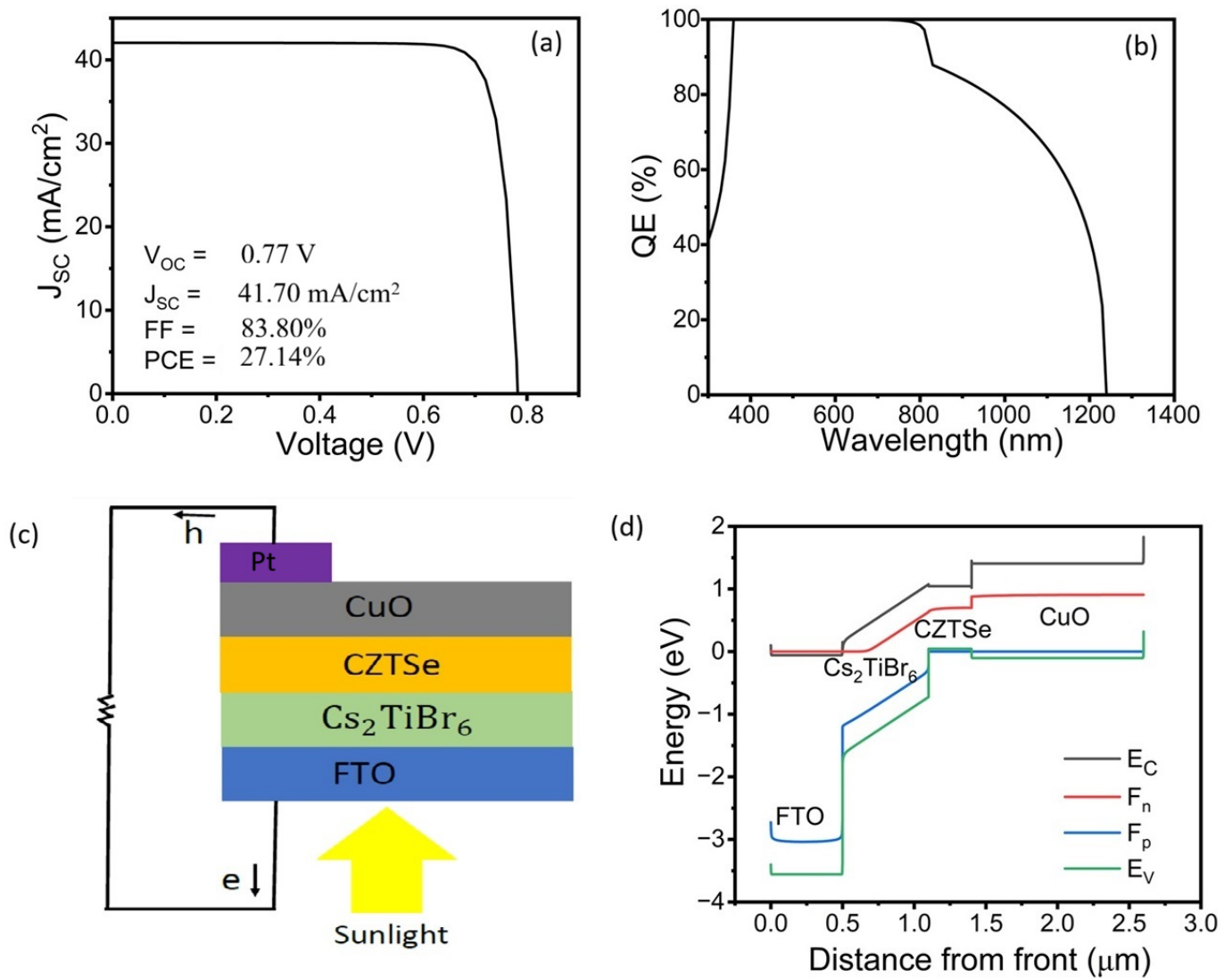


Figure 25: J-V curve of the optimized ETL-free PSC, (b) Associated QE curves, (c) Schematic of the ETL-free design, (d) Energy band diagram of the ETL-free cell.

modestly with thickness, dark saturation current (J_0) also increases slightly due to increased recombination volume and resistive losses. Because of the logarithmic dependence, further increases in thickness do not significantly change V_{oc} , resulting in a plateau at 0.64 V.

$$V_{oc} = \frac{nkT}{q} \ln \left(\frac{J_{ph}}{J_0} + 1 \right), \quad (7)$$

where J_{ph} is the photogenerated current, J_0 the dark saturation current, n the ideality factor, q is electron charge, k is Boltzmann constant, and T is temperature.

The FF progressively diminishes with increasing thickness due to two main factors: heightened series resistance and augmented recombination under forward bias. The thicker HTL results in additional resistive losses, which in turn lowers the slope of the J-V curve close to the maximum power point. Furthermore, the increased recombination occurring under high in-

jection conditions raises the effective ideality factor, which contributes to the reduction of the FF. Despite this gradual decline in FF, the enhancement in J_{sc} prevails, resulting in a continuous rise in PCE (11.13–18.81%). Nevertheless, the incremental gain in efficiency becomes minimal beyond thickness of 0.48 μ m, suggesting that the device is nearing its transport-limited regime.

The thickness of 0.3 μ m will be used as the optimal value for the optimized solar cell. This moderate thickness produced a reasonable PCE value (17.31%), suggesting that it is adequate for the optimized device. It should be noted that a moderate thickness is appropriate to ensure device simplicity and cost-effectiveness.

3.5. Influence of CuO HTL thickness

Figures 10 and 11 depicts the influence of CuO HTL thickness on the device performance. An increase in CuO thick-

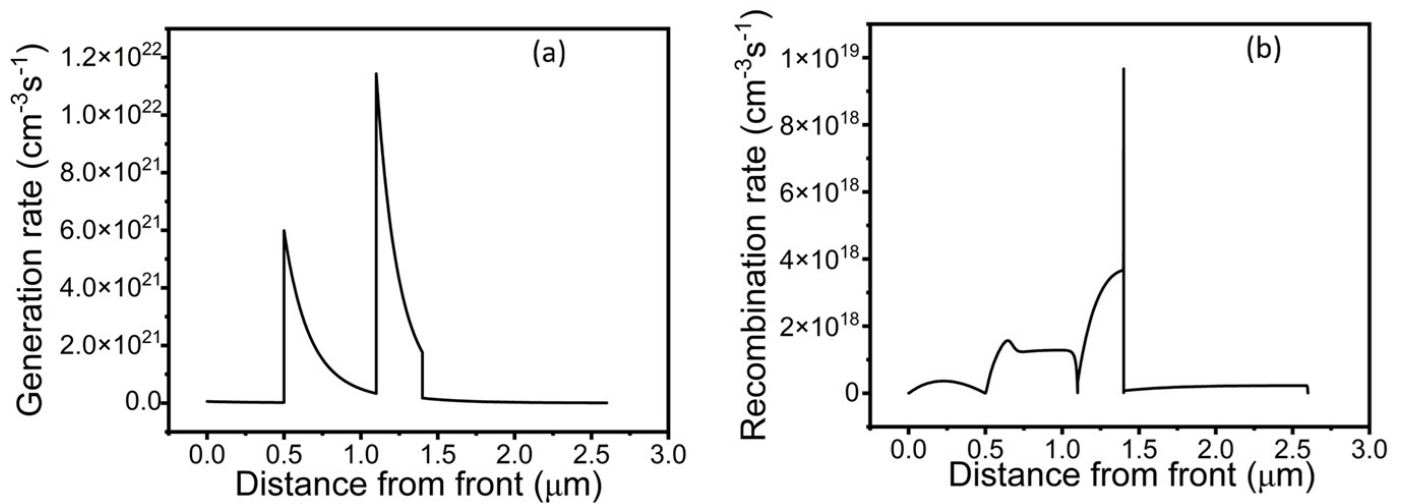


Figure 26: (a) Carrier generation rate for the ETL-free cell, (b) Carrier recombination rate for the ETL-free PSC.

ness (0.20 – 1.20 μm) produces a negligible increase in V_{OC} (0.62 – 0.64 V), while the J_{SC} improves significantly (30.70 – 33.87 mA/cm^2). The FF demonstrates a gradual decline (67.74 – 63.99%), leading to a substantial increase in PCE (12.99 – 13.77%). These results show a delicate balance between reduced interfacial recombination and enhanced charge extraction, and an increase in transport resistance. The boost in J_{SC} with increase CuO HTL thickness suggests that a thicker CuO HTL improves hole transport and suppresses back-contact recombination. CuO has a relatively deep E_{C} (–5.5 eV) and high work function (5.3 – 5.4 eV), which facilitate hole extraction from the underlying CZTSe and blocks electron backflow from the absorber toward the metallic.

Contact between thinner ($\leq 0.2 \mu\text{m}$) CuO HTL with the Ni electrode can allow electron tunneling or recombination through metal-induced gap states and interfacial defects. Increasing the thickness (0.6 – 1.0 μm) forms a more continuous, defect-tolerant barrier that mitigated such recombination channels to allow better charge selectivity and higher J_{SC} . This effect accounts for the steady improvement in J_{SC} and the slight increase in V_{OC} . Also, the increase in J_{SC} can be traced to an improvement in QE between 500–830 nm wavelength (Figure 11b), suggesting improved photon absorption and carrier generation. The small increase in V_{OC} suggests a moderate reduction in non-radiative recombination at the CuO/Ni interface with increased CuO thickness, which better isolates the absorber from the Ni electrode. The FF decreases progressively with increased CuO thickness due to enhanced series resistance in the CuO HTL. This is because the resistivity of CuO is relatively high ($10^3 - 10^4 \Omega\cdot\text{cm}$) due to low hole mobility of $0.1 \text{ cm}^2/\text{V}\cdot\text{s}$ and acceptor concentration of 10^{16} cm^{-3} . Charge transport through CuO became more resistive with increased CuO thickness, leading to a reduction in FF. This behavior agrees with experimental reports, which show that excessive CuO thickness can increase the transport path length, resulting to reduced carrier extraction speed and increased series resistance [35]. Therefore, while the thicker CuO layer

improved interface passivation, it also introduced a balance between selectivity and resistivity. The optimal CuO thickness for this device was identified between 0.8–1.0 μm , where the PCE reaches its maximum (13.75%), achieving a balance between interfacial passivation and efficient charge transport.

CuO offers superior thermal and environmental stability, making it a viable alternative to organic HTLs such as spiro-OMeTAD and P₃HT in PSCs. Further performance improvements in CuO can be achieved by increasing its conductivity through p-type doping with Ni, Li, Na, or oxygen stoichiometry tuning [36]. In addition, interface engineering by inserting an ultrathin CZTS or MoO₃ interlayer can further enhance energy-level matching and reduce series resistance, potentially leading to efficiencies above 15% for this device configuration.

3.6. Defect density of CeO_x ETL

The effect of bulk defect density in the CeO_x ETL is evaluated by sweeping defect density from 2×10^{14} to $1 \times 10^{15} \text{ cm}^{-3}$ (Figures 12 and 13a). All performance metrics remain invariant, where V_{OC} , J_{SC} , FF and PCE stay fixed at, 0.62 V, 30.70 mA/cm^2 , 67.74%, and 12.99%, respectively. This thickness- and performance-insensitivity of the CeO_x bulk traps is consistent with (i) favorable band alignment at the $\text{CeO}_x/\text{Cs}_2\text{TiBr}_6$ interface, (ii) strong n-type conduction in the ETL that suppressed hole populations, and (iii) the reason that device recombination is constrained by interfacial properties, rather than ETL-bulk-limited.

The device performance does not change within the tested defect window because the ΔE_{C} between CeO_x and Cs_2TiBr_6 is small, therefore electron extraction at the front interface is not based on bulk transport through the ETL. CeO_x has been reported to operate as a low-loss, low-recombination ETL in planar PSCs when processed appropriately [37].

The invariance in performance metrics observed here should not be interpreted as universal. CeO_x bulk defects would become performance-relevant if (i) the ETL is made very thin been dominated by pinholes or shunts, (ii) the donor density or

electron mobility in CeO_x is much lower to raise series resistance so that trap-assisted transport becomes rate-limiting, or (iii) the interface defect density at $\text{CeO}_x/\text{Cs}_2\text{TiBr}_6$ increases to couple ETL bulk states with interfacial recombination channels. In such scenarios, both V_{OC} and FF are expected to deteriorate as defect density increases [38].

3.7. Defect density of absorber

Figures 13b, 14 illustrates effect of bulk defect density of the Cs_2TiBr_6 absorber layer on PV behavior of the device. The defect density was varied from 10^{12} to 10^{15} cm^{-3} . The V_{OC} , J_{SC} , FF, and PCE remains constant at 0.62 V, 30.70 mA/cm^2 , ~67.90% and ~13.0%, respectively across the defect range of 10^{12} to 10^{14} cm^{-3} , indicating minimal sensitivity to moderate traps. However, a further increase to 10^{15} cm^{-3} results in a measurable drop in performance as FF declines to 66.32%, PCE decreases to 12.63%, and a slight reduction in J_{SC} to 30.62 mA/cm^2 is observed. These results suggest that, Cs_2TiBr_6 exhibit notable defect tolerance at lower trap densities, but excessive bulk defects lead to deterioration of charge transport and collection efficiency.

Defects within the Cs_2TiBr_6 bulk material primarily serve as SRH recombination centers that reduce the effective carrier lifetime (τ_{SRH}), according to Eq. 8.

$$\tau_{SRH} = \frac{1}{\sigma v_{it} N_t}, \quad (8)$$

where σ is the capture cross-section, v_{it} is carrier thermal velocity, N_t is defect density. Carrier lifetime and diffusion length ($L = \sqrt{D\tau}$) decreases as defect density increases, resulting to enhanced non-radiative recombination losses.

For defect density $\leq 10^{14} \text{ cm}^{-3}$, the effective diffusion length in Cs_2TiBr_6 remains significantly larger than the absorber thickness (0.5 μm), ensuring efficient carrier extraction at both interfaces. Therefore, recombination may be affected by interface traps, because variations in bulk traps does not substantially alter V_{OC} or J_{SC} [12]. However, higher bulk defect density (10^{15} cm^{-3}) results in competition between SRH recombination and interfacial processes, causing carrier collection loss and reduced FF, and consequently reduces PCE [12].

The results reveal that the Cs_2TiBr_6 has a wide defect tolerance up to 10^{14} cm^{-3} , beyond which impairment of charge transport and PCE began to occur. This tolerance comes from the high dielectric constant (Table 1) and the indirect nature of its bandgap, both of which mitigate Coulombic recombination by screening trap potentials and promoting phonon-assisted carrier transport. In practice, high PCE can be sustained at higher defect densities through strategies such as defect passivation, stoichiometric optimization, and halide compensation [33].

3.8. Impact of defect density of CZTSe HTL

Figures 13c and 15 displays effects of bulk defect density ($2 \times 10^{13} - 1 \times 10^{14} \text{ cm}^{-3}$) of CZTSe HTL on device performance. The device shows impressive defect tolerance. The J_{SC} FF remains steady at 30.70 mA/cm^2 and FF fluctuates marginally between 67.59 – 67.74%. Meanwhile, the PCE declines slightly

from 13.08% to 12.99%, mainly due to a small drop in V_{OC} (0.63 – 0.62 V) at the highest defect level. The weak dependence of device performance on defect density of the CZTSe layer suggests that recombination in the HTL has no significant effect on charge collection. Since CZTSe primarily acts as a hole-selective transport layer and is positioned after the absorber layer where photogeneration occurs, the concentration of minority carriers in this layer is naturally low. As a result, any increases in defect-assisted SRH recombination have little impact on current extraction and transport, leading to stable values for J_{SC} and FF.

The slight decrease in V_{OC} with rising defect density is linked to a small uptick in recombination near the $\text{Cs}_2\text{TiBr}_6/\text{CZTSe}$ interface, which causes a modest rise in the dark saturation current (J_0), according to Eq. 7 [34]. However, this effect is countered by the favorable band alignment between Cs_2TiBr_6 and CZTSe, which creates a minimal ΔE_C and facilitates efficient hole transport while reducing electron leakage. Additionally, the relatively high hole mobility of CZTSe, combine with a high-work-function CuO overlayer, helps to maintain low series resistance and stable performance. Higher defect concentrations slightly enhance minority-carrier recombination near the $\text{Cs}_2\text{TiBr}_6/\text{CZTSe}$ interface, tending to reduce the quasi-Fermi level splitting.

3.9. Influence of defect density of CuO layer

Figures 13d and 15 illustrates the impact of defect density of the CuO layer on device performance. The PV metrics stayed unchanged with rising trap density ($2 \times 10^{13} - 1 \times 10^{14} \text{ cm}^{-3}$), where V_{OC} , J_{SC} , FF and PCE remained fixed at 0.62 V, 30.70 mA/cm^2 , 67.74%, and 12.99%. This consistent performance suggests that the operation of the device is not hindered by bulk SRH recombination in the CuO layer.

The lack of sensitivity to CuO bulk defects can be traced to the fundamental role CuO plays in the device setup. As a p-type, high-work-function contact layer that is placed in contact with the contact, CuO has a very low concentration of minority carriers (electrons) due to less light reaching it. Therefore, even when defect density is increased, it does not really boost bulk recombination or the J_0 , which keeps V_{OC} stable [10]. In addition, the main function of transporting holes and blocking electrons is already executed by the inner CZTSe HTL. CuO mainly helps align the Fermi level with the metal contact and reduces the impact of metal-induced gap states [36]. Since most of the photogeneration and carrier transport happens in the absorber and CZTSe layers, charge carriers do not linger in CuO for long, making its bulk defects mostly inactive.

This behavior is further supported by the favorable band alignment at the rear contact. The stepwise valence-band energy from Cs_2TiBr_6 to CZTSe to CuO creates a pathway for efficient hole extraction, while the deep conduction band of CuO acts as a strong barrier to prevent electron leakage toward the rear metal contact [21, 36].

3.10. Influence of acceptor doping in CZTSe layer

The acceptor doping concentration in the CZTSe hole transport layer (HTL) is crucial for managing charge extrac-

tion, interfacial energetics, and recombination dynamics solar cells [37](Table 5). An increase in acceptor concentrations ($10^{15} - 10^{18} \text{ cm}^{-3}$) produce a significant boost in PCE (12.99 – 16.00%). Interestingly, the J_{SC} decrease only slightly. Raising the acceptor doping moves the Fermi level of the p-type CZTSe HTL closer to its valence band maximum. This adjustment enhances band bending and amplifies the built-in electric field at the $\text{Cs}_2\text{TiBr}_6/\text{CZTSe}$ interface, which is the main interface for hole extraction. The stronger internal electric field aids in the efficient separation of photogenerated electron-hole pairs in the Cs_2TiBr_6 absorber and encourages the directional transport of holes toward the back contact (Ni). As a result, recombination losses at the heterointerface are minimized, leading to better device performance.

In more details, an increase in the acceptor doping in the CZTSe HTL produces a significant increase in electrical conductivity. This change helps lower the series resistance of the device and enhances hole transport across the CZTSe/CuO/Ni stack. This leads to better carrier extraction efficiency, which directly leads to an increase in the FF and PCE. Additionally, the improved band alignment between CZTSe and the high-work-function Ni electrode (5.1 eV) allows for more effective ohmic hole collection, reducing those unwanted contact-related energy barriers. By contrast, a slight decrease in J_{SC} is observed upon increasing the acceptor concentration. This can be ascribed to increased ionized impurity scattering and more recombination happening in the heavily doped CZTSe HTL. When doping levels get high, the depletion width at the $\text{Cs}_2\text{TiBr}_6/\text{CZTSe}$ interface narrows a bit Eq. 9, which slightly limits the space available for separating photogenerated carriers. Additionally, high hole concentrations might lead to more Auger recombination and free-carrier absorption losses, which could cap the photocurrent. However, the drop in J_{SC} is minimal (3%), suggesting that the impact of increased doping is more beneficial for charge extraction than harmful to carrier generation.

$$W_p = \sqrt{\frac{1}{N_A}}, \quad (9)$$

where W_p is depletion width, N_A is acceptor carrier concentration.

3.11. Effect of acceptor doping in CuO layer

Elevating the acceptor doping concentration ($10^{15} - 10^{18} \text{ cm}^{-3}$) in the CuO HTL clearly enhances the PV performance of the solar cell (Figure 16). This is evident from the consistent improvements across all key device parameters. The V_{OC} rise from 0.62 to 0.67 V, the J_{SC} increase from 30.70 to 31.24 mA/cm^2 , and a significant boost in the FF from 67.74 to 76.58%. Also, the PCE boosts from 12.99 to 16.10%. These trends suggest that higher CuO doping leads to better charge extraction and fewer electrical losses.

An increase in the acceptor doping in the p-type CuO HTL shifts its Fermi level closer to the valence band. This adjustment improves the band alignment at both the CZTSe/CuO heterointerface and the CuO/Ni back contact. The built-in electric

field at the CZTSe/CuO junction is enhanced with this better alignment, which helps in efficiently extracting holes from the absorber region while effectively blocking electrons. The improved electrostatic field and lower interfacial energy barriers reduce interfacial recombination, resulting in a greater quasi-Fermi level splitting and the observed increase in V_{OC} .

In addition, boosting the acceptor doping increases the electrical conductivity of the CuO HTL. This not only reduce series resistance but also enhances hole transport towards the high-work-function Ni electrode. The decline in resistive losses plays a crucial role in the noticeable increase in FF, while better carrier collection efficiency brings about a steady, albeit modest, rise in J_{SC} .

3.12. Impact of defect density of $\text{CeO}_x/\text{Cs}_2\text{TiBr}_6$ interface

Figures 17 depicts the influence of defect density of the $\text{CeO}_x/\text{Cs}_2\text{TiBr}_6$ interface ($1 \times 10^{10} - 1 \times 10^{17} \text{ cm}^{-2}$) on performance of the PSC. The device performance stays unchanged in the interface defect density range of 10^{10} to 10^{14} cm^{-2} , indicating that the cell operates in a regime where interface SRH recombination is not the dominant loss mechanism. Therefore, the V_{OC} and J_{SC} stayed around 0.62 V and 30.70 mA/cm^2 , respectively, while PCE hovered around 12.99%. The only noticeable change was a minor drop in FF (67.75 – 67.68%) at the interface trap density of 10^{14} cm^{-2} . However, an increase in trap density beyond 10^{14} cm^{-2} resulted in an increase in the effective interfacial recombination strength, which is sufficient for the ETL/absorber interface to become a major recombination pathway. This transition primarily reduced the FF (67.68 – 61.16%) due to enhanced recombination current, and also lowered J_{SC} (30.70 – 29.22 mA/cm^2) by reducing carrier collection. V_{OC} demonstrated only a modest reduction at the highest defect density because it depends logarithmically on recombination current. Meanwhile, the PCE degraded significantly from 12.98% at 10^{14} cm^{-2} to 10.94% at 10^{17} cm^{-2} .

In practice, the device performance can be improved by optimizing by annealing CeO_x in mild O_2 to reduce excessive oxygen vacancies that act as recombination centers, and adding an ultrathin passivation layer (1 - 5 nm) of TiO_2 or SnO between CeO_x and Cs_2TiBr_6 .

3.13. Effect of varied defect density of the absorber/CZTSe and CZTSe/Cuo interfaces

The contour plots (Figure 18) reveals that the PSC is more sensitive to defects at the Absorber/CZTSe interface than at the CZTSe/CuO interface. In both cases, increasing interface defect trap degrades device performance, but the magnitude of deterioration is clearly larger for the Absorber/CZTSe interface. Raising the defect density at the Absorber/CZTSe interface from 10^{10} to 10^{13} cm^{-2} reduces the V_{OC} from 0.66 to 0.62 V (Figures 18a), J_{SC} from 30.71 to 30.70 mA/cm^2 (Figures 18b and 19a), FF from 69.84 to 67.74% (Figure 18c), and the PCE from 14.11 to 12.99% (Figure 18d). This implies that the PCE dips by about 1.12% points, which is the largest loss observed. The contour maps confirm this strong dependence by showing a rapid shift in the performance region from high values at low

Table 5: Impact of acceptor doping concentration of CZTSe on PV performance.

Acceptor of doping concentration (cm ⁻³)	Voc (V)	Jsc (mA/cm ²)	FF (%)	PCE (%)
10 ¹⁵	0.62	30.70	67.74	12.99
10 ¹⁶	0.62	30.70	67.74	12.99
10 ¹⁷	-	30.31	-	14.43
10 ¹⁸	-	30.02	-	16.00

defect density to much lower values as the Absorber/CZTSe interface turns more defective. This characteristic indicates that this interface is the dominant recombination-active interface in the device. Since carriers are generated in the absorber and holes must be transferred into CZTSe, a high density of interface traps boosts SRH recombination, reduces quasi-Fermi level splitting, and suppresses both V_{OC} and FF. The small decline in J_{SC} (Figures 18 and 19a) suggests that carrier generation remains essentially constant, but carrier collection becomes slightly less efficient when recombination increases.

The effect is weaker at the CZTSe/CuO interface (Figures 18 and 19b). An increase in the interface defect density changes reduces V_{OC} from 0.64 to 0.62 V (Figure 18a), while J_{SC} remains constant at 30.70 mA/cm² (Figures 18b and 19b). The PCE declines only slightly from 13.13 to 12.99% (Figure 18d). Although the FF exhibits a slight increase from 67.00 to 67.74% (Figure 18c), the PCE still deteriorates because the loss in V_{OC} is significant. This contour plots supports this behaviour by showing a gentler gradient along the CZTSe/CuO axis compared with the absorber/CZTSe axis confirms that the absorber/CZTSe interface has a stronger impact on device performance than the CZTSe/CuO interface

3.14. Impact of back contact metal work function

The work function of the metal back contact is crucial for creating a sufficient built-in potential and facilitating effective hole extraction in PSC [39]. This impact is assessed by varying the metal work function from 5.10 to 5.90 eV (Table 6 and Figure 20), while keeping all other parameters and illumination conditions constant. An increase in the work function from 5.10 to 5.50 eV produces a significant improvement in all PV performance metrics. Specifically, the V_{OC} rise from 0.62 to 0.66 V, the J_{SC} increases from 30.70 to 32.48 mA/cm², and the FF sees a substantial boost from 67.74 to 78.42%. These enhancements lead to a notable increase in PCE (12.99 – 16.73%). However, further increases in the work function beyond approximately 5.5 eV yield minimal additional improvements, indicating that performance has reached a saturation point.

At a low work function of around 5.10 eV, there is a significant energetic mismatch between the metal Fermi level and the valence-band maximum of the CZTSe/CuO bilayer. This mismatch results in a Schottky-type, non-ohmic rear contact characterized by a positive hole barrier height. Such a barrier hinders hole extraction, leads to carrier accumulation near the back interface, and increases interfacial recombination [44]. Consequently, quasi-Fermi-level pinning and heightened series resistance reduce both the V_{OC} and FF, while the J_{SC} may also be suppressed due to recombination losses at the rear contact.

Boosting the work function to around 5.5 eV significantly enhances the energy-level alignment between the CuO valence band and the metal Fermi level. This adjustment lowers the hole extraction barrier, effectively turning the CuO/Ni interface into an ohmic-like contact. With this better alignment, hole transport and extraction become more efficient, non-radiative recombination at the rear interface is minimized, and resistive losses are cut down. The increase in V_{OC} can be linked to the reduced rear-interface recombination, while the notable improvement in FF highlights the reduction in series resistance and the enhancement in PCE. The slight rise in J_{SC} is due to more effective charge collection and a more even distribution of the internal electric field across the absorber.

When work functions hit 5.6 eV or higher, all performance metrics level off, suggesting that the rear contact has reached the ohmic threshold, with a minimal or even negative hole barrier height. In this scenario, hole extraction is not a limiting factor anymore, and the elevated work function also helps to curb electron leakage towards the back contact. The observed plateau in PCE between 5.6 and 5.7 eV indicates that device performance is no longer limited by the back-contact energetics but rather by the inherent quality of the absorber and the remaining interfaces.

The contact selectivity can be explained by Eqs. 10 and 11 [45, 46].

$$\phi_{b,p} = E_{V,CuO} - (-\phi_M), \quad (10)$$

where

$$E_{V,CuO} = \chi_{CuO} + E_{g,CuO} \quad (\text{vs. vacuum}) \quad (11)$$

and $E_{V,CuO}$ is valence band maximum of CuO, χ_{CuO} is electron affinity of CuO, $E_{g,CuO}$ is bandgap of CuO, ϕ_M metal work function of back contact, $\phi_{b,p}$ is hole barrier height.

3.15. Effect of series resistance

The main contributors to series resistance in perovskite solar cells are the sheet resistance of the transparent conductive oxide, the bulk resistance of the transport layers, interfacial contact resistance, and the resistance of the metal electrodes. These resistive elements cause internal voltage drops when a forward bias is applied, which ultimately lowers the FF and the PCE [47, 48]. Figures 21a, b reveals that raising the series resistance (0 – 5 Ωcm^2) significantly reduce the FF (67.74 – 48.16%) because it produces a voltage drop ($\Delta V = J.R_s$), which affects the shape of the J–V curve and shifts the maximum-power point to lower power. In contrast, J_{SC} remains essentially constant

Table 6: Variation of PV performance with back contact metal work function.

Metal	Work function (eV) [26, 40–43]	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	PCE (%)
Ni	5.10	0.62	30.70	67.74	12.99
Mo	5.22	0.65	30.88	76.86	15.49
Au	5.50	0.66	32.43	78.41	16.70
Pd	5.60	0.66	32.48	78.42	16.73
Pt	5.70	0.66	32.48	78.42	16.73

(~30.70 mA/cm²) because J_{SC} is primarily generation and collection limited, and V_{OC} remains unchanged because there is no resistive drop at open circuit (J = 0). Therefore, the decline in PCE with increasing series resistance is controlled by the decrease in FF, which highlight the importance of minimizing contact and layer resistances to boost performance. This finding agrees with the standard diode model (12) [26, 44], which indicates that series resistance has a substantial impact on FF and PCE (12.99 – 9.23%), while leaving V_{OC} (0.62 V) and J_{SC} relatively unchanged within moderate range [49].

$$J = J_{ph} - J_0 \left[\exp \left(\frac{q(V + JR_s)}{nkT} \right) - 1 \right] - \frac{V + JR_s}{R_{sh}}, \quad (12)$$

where J is output current, J_{ph} is photocurrent density, J_0 is reverse current, R_s denote series resistance, R_{sh} represent shunt resistance, T is temperature, V is applied voltage, k is Boltzmann constant, q is charge, and n is ideality factor. At short circuit ($V = 0$ V), the term JR_s is small compared with kT/q and the potential drop across R_s is negligible, so J_{SC} is essentially independent of R_s . This supports the constant J_{SC} values in this simulation. At open circuit ($J = 0$), the R_s term vanishes, and V_{OC} is determined mainly by the ratio of the J_{ph} and the recombination current in the device, again supporting the constant value of V_{OC} for all values of R_s .

3.16. Influence of shunt resistance

A rise in shunt resistance often leads to power losses, because of problems that occur during manufacturing. In solar cell, power losses happen when shunt resistance is low, as this creates an alternative path for the current generated by light [48]. Shunt resistance occurs in real cells by imperfect coverage, pinholes, edge leakage, conductive filaments, or highly defective grain-boundary paths. The shunt term can be described by Eq. 13 [26] where V is voltage, J_{sh} is shunt current, R_{sh} and R_s denote shunt and series resistances, respectively.

$$J_{sh} = \frac{V + JR_s}{R_{sh}}. \quad (13)$$

The net terminal current should be zero when the circuit is open. If the shunt resistance is low, a leakage current even at moderate voltages would be noticed, which means the device hits that zero-current state at a much lower voltage. Hence V_{OC} drops slightly (0.62–0.59 V) with decreasing resistance (10⁵ - 10¹ Ωcm²) (Figures 12c,d). The leakage provides an easy recombination path that lowers the quasi-Fermi level splitting. FF increases significantly (60.72 – 67.74%) as shunt resistance increases because shunting strongly distorts the shape

of the J–V curve near the maximum power point, where the operating voltage is substantial. An increase in shunt resistance led to negligible leakage, causing the J–V curve to recover its ideal diode shape, while the FF increases to its high-value limit (67.74%). The J_{SC} remains constant throughout the tested range because $V = 0$ and the $J_{sh} = 0/R_{sh} = 0$ under short circuit operation, therefore, the J_{sh} is controlled mainly by photo-generation and collection, not by shunt leakage. This makes the J_{SC} to remain steady at 30.70 mA/cm² across the sweep. The PCE increase (10.94 – 12.99%) can be ascribed to the increase in V_{OC} and FF, although J_{SC} remains unchanged. Shunt resistance of greater than 10³ Ωcm² greatly suppressed leakage, so that further increases produce only minor gains, causing the observed saturation of PCE (12.97 – 12.99%).

3.17. Performance of the optimized CZTSe/CuO double HTL-based PSC

Table 7 presents the new optimal parameters derived during the prototype simulation. Any parameter not mentioned in Table 7 remains the same as in the prototype cell. The relatively low values of optimized interface and bulk defect density are within the range commonly reported for experimentally realized high-quality thin-film and perovskite photovoltaic materials and are frequently adopted in SCAPS-1D studies to represent low-defect devices. These values of interface and bulk defect density are supported by the sources [40, 51–56] and [40, 53, 55–59], respectively.

The optimized FTO/CeO_x/Cs₂TiBr₆/CZTSe/CuO/Pt device showcases impressive PV performance, as shown in Figure 22. With a high V_{OC} of 0.77 V, a substantial J_{SC} of 41.69 mA/cm², and an outstanding FF of 83.78%, this device achieves a PCE of 27.12%, which is higher than the PCE of the prototype counterpart cell (FTO/CeO_x/Cs₂TiBr₆/CZTSe/CuO/Ni) by 2.09-fold. This indicates that the cell excels in generating, separating, and extracting charge throughout the device stack. These performance metrics suggest an ideal diode behavior, with negligible resistive and recombination losses. Interestingly, aside the extreme J_{SC} value, the other recorded PV parameters are consistent with the Shockley-Queisser (SQ) limit of V_{OC} = 1.496 V, J_{SC} = 19.65 mA/cm², FF = 91.40%, and PCE = ~27% for a single-junction solar cell using a perovskite absorber with a bandgap of 1.8 eV [60, 61].

A significant factor contributing to this performance is the switch from a Ni back contact to Pt, which boasts a high work function of 5.7 eV. This work function closely matches the valence band maximum of the p-type CuO HTL, creating a quasi-ohmic or fully ohmic back contact for holes. Consequently,

Table 7: Optimal parameters derived from the prototype solar cell.

New optimized parameters	CZTSe	CuO	Cs ₂ TiBr ₆	CeO _x	All interfaces
Thickness (μm)	0.6	1.2	0.6	0.1	-
N_D (cm^{-3})	-	-	-	-	-
N_A (cm^{-3})	10^{18}	10^{18}	-	-	-
N_t (cm^{-3}) for bulk	-	-	10^{14}	-	-
N_{it} (cm^{-3}) for interfaces	-	-	-	-	10^{10}

the extraction of holes from the CuO layer into the Pt electrode is highly efficient, with virtually no energy barrier. This enhanced back-contact selectivity reduces carrier accumulation and recombination at the CuO/Pt interface, significantly boosting the quasi-Fermi level splitting and, in turn, increasing both V_{OC} and FF.

The impressive J_{SC} (41.69 mA/cm^2) is supported by the outstanding spectral response highlighted in the QE curve (Figures 22b, c). A nearly perfect QE can be seen across a wide range of wavelengths, from the visible spectrum all the way into the near-infrared. This suggests that the CZTSe layer played dual roles of serving as a HTL and concurrently acting as the second absorber layer. Therefore, the optimized device should be interpreted as a Cs₂TiBr₆/CZTSe photoactive heterostructure (or dual-absorber-like architecture) rather than a conventional single-absorber Cs₂TiBr₆ solar cell. This can be seen in the high QE and the absorption edge in which the narrow-bandgap CZTSe extends the optical absorption into the near-infrared region, matching with the bandgap of 1.0 eV and wavelength of 1240 nm. The carrier generation profile clearly indicate that the generation rate is higher in the CZTSe layer (Figure 23a). These agree with the significant boost in J_{SC} up to 45.54 mA/cm^2 as reflected in the substantial increase in QE with an increase in CZTSe film thickness (Figures 8, 9). The Cs₂TiBr₆ perovskite absorber contributed less to J_{SC} upon film thickness increase because photon absorption and carrier generation was restricted within wavelength of $\leq 689 \text{ nm}$ (Figures 6, 7, 22c). These explains why the J_{SC} value exceed the SQ limit (of 19.65 mA/cm^2) for a solar cell utilizing Cs₂TiBr₆ perovskite as the single absorber layer. Nevertheless, this plausible J_{SC} value is consistent with the SQ limit of 48.22 mA/cm^2 for a solar cell using CZTSe absorber layer with a bandgap of 1.0 eV [1, 2]. It should be noted that CZTSe has been used as a single absorber layer in PV solar cells to record high PCEs [62–64]

Table 8 provides a comparison of the PV performances between the current device and other Cs₂TiBr₆-based and the ETL-assisted PSCs. It can be seen that the current device achieves an impressive PCE value of 27.12%. This value is about 0.59% greater than the highest value (26.96%) [12] reported for Cs₂TiBr₆-based PSC in the literature. This success can be attributed to the excellent band alignment between CZTSe and CuO. To emphasize, the back interface (CZTSe/CuO) played a crucial role in enhancing hole selectivity and improving electron blocking, which ultimately leads to more effective photocarrier extraction. Interestingly, the current optimized devices were simulated using input parameter values that are similar with those employed by Kar-

maker *et al.* to record the PCE of 26.96% for the Cs₂TiBr₆-based PSC [12]. The workers simulated the optimized device using acceptor and donor doping concentrations of 10^{19} and 10^{18} cm^{-3} for the ETL and HTL, respectively, interface and bulk defect densities of 10^{10} cm^{-2} and 10^{13} cm^{-3} , respectively [12]. Importantly, the current findings demonstrates that the proposed FTO/Cs₂TiBr₆/CZTSe/CuO/Pt ETL-free architecture is an alternative to obtain a high PCE of 27.12% (Table 7) in the absence of the CuSbS₂ and ZnO materials employed by Karmaker *et al.* To record a PCE of 26.96% from the Pt/CuSbS₂/Cs₂TiBr₆/ZnO/FTO configuration.

3.18. Carrier generation and recombination profiles

The spatial profiles of how carriers are generated and recombined in the optimized FTO/CeO_x/Cs₂TiBr₆/CZTSe/CuO/Pt solar cell explains why it performs well in terms of PV efficiency. Carrier generation mainly takes place in the Cs₂TiBr₆ absorber layer, thanks to its ideal bandgap of 1.8 eV, which allows for effective absorption of visible light (Figure 23a). Moderate carrier generation occurs at $0.6 \mu\text{m}$ (at the front of Cs₂TiBr₆), and decreases as light penetrates into the absorber. This is followed by a sharp generation in the CZTSe layer ($1.2 \mu\text{m}$), and decreases towards the back of the PSC because most of the light was absorbed by the $0.6 \mu\text{m}$ thick CZTSe layer. Therefore, the CZTSe layer acted as the second absorber to harvest photons in the near-infrared (Figures 8, 9, 23a). The higher carrier generation rate in the CZTSe layer (Figure 23a) suggest that this layer served dual role in the device architecture by acting as HTL, and concurrently acting as the most active absorber layer to contribute to carrier generation to support the plausible J_{SC} value of $\sim 42 \text{ mA/cm}^2$. Photons incident from the FTO side excite electrons from the valence band to the conduction bands of the Cs₂TiBr₆ and CZTSe layers, creating electron-hole pairs. The CeO_x ETL is designed to selectively extract electrons while blocking holes, which helps to reduce carrier loss at the front interface. Meanwhile, the CZTSe/CuO dual HTL aid in collecting holes and prevent electrons from flowing back toward the rear electrode.

Recombination in the cell (Figure 23b) primarily occurs in the bulk of the CZTSe layer and at the interfaces. The bulk recombination is kept in check due to the moderate defect density (10^{14} cm^{-3}), which allows most of the photogenerated carriers to reach the transport layers. Interface recombination is significantly reduced through defect engineering, with the interface trap density fine-tuned to 10^{10} cm^{-2} at the various interfaces. Additionally, the high carrier mobilities in the ETL and HTL

Table 8: Comparison of performance metrics between experimental and simulated Cs₂TiBr₆/CZTSe photoactive heterojunction PSCs.

Perovskite solar cell	Nature of electron transport	Preparation method	PCE (%), FF (%), J _{sc} (mA/cm ²), V _{oc} (V)	references
FTO/CeO _x /Cs ₂ TiBr ₆ /CZTSe/CuO/Pt	ETL-based	SCAPS-1D	27.12, 83.78, 41.69, 0.77	This work
FTO/Cs ₂ TiBr ₆ /CZTSe/CuO/Pt	ETL-free	SCAPS-1D	27.14, 83.80, 41.70, 0.77	This work
FTO/TiO ₂ /Cs ₂ TiBr ₆ /Au	ETL-based	Experiment	2.34, NA, NA, 0.89	[67]
FTO/TiO ₂ /Co ₆ O/Cs ₂ TiBr ₆ /P ₃ HT/Au	ETL-based	Experiment	3.28, 56.4, 5.69, 1.02	[11]
Al/FTO/ZnSe/Cs ₂ TiBr ₆ /Cu ₂ O/Os	ETL-based	SCAPS-1D	23.84, 83.34, 20.53, 1.39	[68]
FTO/CeO _x /Cs ₂ TiBr ₆ /CZTS/P ₃ HT/Au	ETL-based	SCAPS-1D	22.61, 80.35, 27.08, 1.04	[10]
Pt/CuSbS ₂ /Cs ₂ TiBr ₆ /ZnO/FTO	ETL-based	SCAPS-1D	26.96, 81.36, 31.63, 1.05	[12]
FTO/SnO ₂ /Cs ₂ TiBr ₆ /CBTS/Au	ETL-based	SCAPS-1D	24.24, 88.9, 20.76, 1.32	[9]
Au/TiO ₂ /Cs ₂ TiBr ₆ /CuI/Au	ETL-based	SCAPS-1D	21.17, 81.42, 32.93, 0.79	[15]
FTO/CdS/Cs ₂ TiBr ₆ /Cu ₂ SbS/Au	ETL-based	SCAPS-1D	23.77, 84.76, 24.39, 1.15	[14]
FTO/TiO ₂ /Cs ₂ TiBr ₆ /MoO ₃ /Au	ETL-based	SCAPS-1D	15.02	[69]
FTO/SnO ₂ /Cs ₂ TiBr ₆ /MoO _x /Au	ETL-based	SCAPS-1D	20.11, 82.17, 16.34, 1.45	[16]
ITO/LBSO/Cs ₂ TiBr ₆ /CNTS/Au	ETL-based	SCAPS-1D	24.82, 82.94, 26.63, 1.12	[13]

ensure that electrons and holes are transported quickly, further decreasing the chances of recombination within the transport layers.

3.19. Effect of sun concentration on PV performance

The study of sunlight concentration in PSCs is crucial because it helps in understand how higher light intensity impacts photocurrent generation, carrier recombination, and the PCE. Metrics such as J_{SC} and power output can be boosted using concentrated light. Also, the thermal and optical limits of the device can be uncovered under concentrated light, and can steer the optimization of material properties and layer design to create high-performance and scalable PSCs [68]. Figure 24 depicts the impact of increasing sun concentration on device performance. The J_{SC} increases from 41.69 to 2416.35 mA/cm² in the sun concentration range of 1 to 50 suns, exhibiting a linear dependence on the concentration ratio (C). Under illumination, the generation rate (G) is proportional to the photon flux, according to 14 [69].

$$G(C) = CG_1, \quad (14)$$

where G_1 is the generation rate at 1 sun. In the absence of transport limitations, J_{SC} takes the form of 15 [69].

$$J_{SC} = q \int_0^W G(C, x) dx \propto C, \quad (15)$$

where q is the elementary charge and W is the absorber thickness. The nearly linear scaling of J_{SC} suggests that carrier collection continues to be effective even at elevated injection levels. There is no significant sublinear behavior detected, indicating that space-charge effects, mobility constraints, or intense Auger recombination do not play a major role within this concentration range. This behavior indicates robust built-in electric fields throughout the heterojunction, elevated carrier mobilities

in the transport layers (CeO_x and CuO), and effective carrier selectivity at both the front and rear contacts.

The V_{OC} increases from 0.77 to 0.92 V with elevating sun concentration. The dependence of V_{OC} on illumination intensity follows Eq. 7. Since J_{SC} ∝ C, the voltage takes a logarithmic dependence in Eq. 16 [70]. The observed rise in V_{OC} indicates that the J₀ remains at a low level, which signifies that non-radiative recombination is suppressed. The moderate incline of the V_{OC} increase implies that recombination is mainly influenced by SRH and radiative processes, rather than significant Auger recombination, which would lead to deviations at elevated carrier densities. The effective carrier selectivity offered by CeO_x and CuO/Pt (high-work-function back contact) likely reduces minority-carrier leakage, thus preserving a low J₀.

$$V_{OC}(C) = \frac{nkT}{q} \ln(C) + \text{constant}, \quad (16)$$

The FF remains high (83.78 – 81.63%) across the entire concentration range, decreasing slightly from. In an ideal diode without resistive losses, the FF depends mainly on V_{OC}. However, in practical devices, series resistance and shunt resistance influence the FF. At high current densities, the voltage drops across the series resistance becomes significant, according to 17 [71]

$$\Delta V_{series} = JR_s. \quad (17)$$

As J rises in proportion to C , the resistive voltage drop also increases, resulting in a rounding of the J-V curve close to the maximum power point and a minor decrease in FF. The gradual and limited degradation of FF suggests low intrinsic series resistance, minimal contact barriers at the FTO/CeO_x and CuO/Pt interfaces, and strong diode quality with restricted shunt leakage. Additionally, at elevated carrier densities, high-level injection may enhance bimolecular and Auger recombination 17 [72], which can subtly modify the curvature of the J-V

characteristics near the maximum power point. However, these effects remain minor within 50 suns.

$$R_{Auger} = C_n n^2 p + C_p n p^2, \quad (18)$$

where n and p are the donor and acceptor carrier densities, respectively.

The PCE increases from 27.12 to 36.10% with increasing suns. Under concentrated illumination, the incident power is given by Eq. 19 [73].

$$P_{in}(C) = C P_{in, 1}. \quad (19)$$

Because of the relationships $J_{SC} \propto C$ (15) and $V_{OC} \propto \ln(C)$ (16), the enhancement in PCE is mainly attributed to the logarithmic increase in V_{OC} , while the FF remains largely unchanged. The initial swift improvement observed between 1 and 20 suns is a result of concurrent increases in J_{SC} and V_{OC} . However, beyond 20 suns, the increase in PCE becomes more gradual due to factors, such as the logarithmic characteristic of V_{OC} , the rise in resistive losses ($J.R_s$), and the potential emergence of high-injection recombination effects. Consequently, the device shifts from a regime limited by photogeneration at low concentrations to one that is mildly influenced by resistance and recombination at higher concentrations.

3.20. PV performance of the ETL-free PSC

Investigating the ETL-free solar cells is important because getting rid of the ETL makes the device design simpler, reduces manufacturing costs, and helps minimize issues like interfacial defects that can cause recombination and unwanted optical losses. Additionally, the ETL-free designs help to directly assess how well the absorber can separate charges, transport them, and align energy levels, which is key for creating stable and scalable PSC [48–50, 65]. ETL-free PSCs have been reported in the literature scoring PCE values, such as 22.0% for single junction [74, 75], and 45.99% for ETL-free tandem solar cell. Experimental studies have reported PCE values, such as PCE of 10.92% [76], 13.60% [67], 20.10% [77], 20.0% [78], and 22.0% [75], supporting the robustness of the ETL-free design.

The ETL-free design (FTO/Cs₂TiBr₆/CZTSe/CuO/Pt) shows a negligible boost in its FF (83.80%) and PCE (27.14%), indicating that its performance is comparable with the ETL-assisted counterpart (Figure 25). This suggests that effective electron extraction is possible without the CeO_x ETL. This can be understood by looking at the interfacial band alignment, transport resistance, and the physics of recombination at the front contact. For the ease of reference, the schematic and energy band diagram of the ETL-free configuration is depicted in Figures 25c,d.

A critical look at the band alignment reveals that the conduction band of Cs₂TiBr₆ aligns nicely with the work function and electron affinity of FTO. This means that electrons can be pulled out efficiently without facing a big energy barrier. Thanks to this quasi-ohmic electron contact, the photo-generated electrons are collected quickly, which helps prevent

charge buildup and cuts down on interfacial recombination. As a result, the V_{OC} stays impressively high at 0.77 V, showing that not having CeO_x does not lead to any extra voltage losses.

Figure 26a demonstrates that the photogeneration profile of the ETL-free device is identical with the ETL-assisted counterpart (Figure 23a), confirming that the removal of CeO_x does not affect optical absorption or carrier generation. More importantly, the recombination rate distributions (Figures 23b, 26b) show that: (i) the dominant recombination occurs within the absorber bulk region in both structures, (ii) there is no pronounced spike in recombination observed at the FTO/Cs₂TiBr₆ interface in the ETL-free device, and (iii) the interfacial recombination peak at the front junction remains comparable between the ETL-assisted and ETL-free configurations. These observations indicate that removal of the CeO_x ETL does not introduce significant front-interface recombination losses. These findings confirm that the FTO/Cs₂TiBr₆ interface does not introduce significant additional recombination pathways when CeO_x is removed, while the primary recombination contribution remains within the Cs₂TiBr₆ absorber. Furthermore, the conduction band offset at FTO/Cs₂TiBr₆ is small (-0.17 eV), enabling efficient electron extraction, and the valence band offset is large (+1.53 eV), providing strong hole blocking. This makes the FTO/Cs₂TiBr₆ interface to inherently function as an electron-selective contact, which explains why the ETL-free device achieves comparable PCE without increased interfacial recombination.

The QE spectrum of the ETL-free device is comparable with the ETL-assisted counterpart, supporting the equivalent value of J_{SC} recorded in both devices. This nearly perfect QE across the visible spectrum shows that photocarrier generation and collection are working well. Also, the lack of short-wavelength QE suppression indicates that there is less parasitic absorption compared to the device that uses CeO_x. Eliminating the optical losses in the ETL leads to more high-energy photons that can reach the absorber, which helps to slightly boost the J_{SC} and PCE.

3.21. Practical implications and modeling limitations

It is important to point out that SCAPS-1D uses a one-dimensional drift-diffusion model, which assumes that the material properties are uniform and that the interfaces are perfectly planar [79–85]. Because of this, the simulation ignores factors like grain boundaries, pinholes, lateral variations, or any non-uniformities in morphology that might often be found in real-world devices [12, 84]. These factors can create extra recombination pathways and add series resistance, which ultimately results in lower practical efficiencies. Therefore, the optimized performance (high PCEs of 27.12 and 27.14% for the ETL-assisted and ETL-free devices, respectively) highlighted in this study are more of a theoretical maximum under ideal conditions, mainly aimed at shedding light on how interface defect density and band alignment influence the proposed devices.

4. Conclusion

In summary, this work has proposed an efficient lead-free FTO/CeO_x/Cs₂TiBr₆/CZTSe/CuO/NiETL-assisted PSC through numerical simulation using SCAPS-1D software. The device was optimized using optimal values of layer thickness, bulk and interface defect density, back contact work function, and doping concentration of the HTLs. The optimized FTO/CeO_x/Cs₂TiBr₆/CZTSe/CuO/Pt ETL-assisted device delivered a PCE, FF, J_{SC}, and V_{OC} of 27.12%, 83.78%, 41.69 mA/cm², and 0.77 V, respectively. Results show an increase in PCE values from 27.12 to 36.10% with rising sunlight concentration from 1 to 50 suns. The counterpart ETL-free design (FTO/Cs₂TiBr₆/CZTSe/CuO/Pt) of the optimized cell yielded a comparable PCE of 27.14%, suggesting that the ETL is dispensable, and its removal leads to a simple and cost-effective design. The ETL-free design for the Cs₂TiBr₆/CZTSe photoactive heterostructure is investigated for the first time, demonstrating that efficient carrier separation and transport were achieved without an ETL under the idealized SCAPS-1D simulation conditions. The PCE, FF and V_{OC} values of the optimized device agrees with the SQ limit for a single-junction solar cell utilizing an absorber with bandgap of 1.8 eV. The impressively high J_{SC} originates from the combined photogeneration in both Cs₂TiBr₆ and CZTSe photoactive layers, where the narrow-bandgap CZTSe layer extends the photoresponse into the near-infrared region and contributes significantly to carrier generation. As a result, the optimized structure is best described as a Cs₂TiBr₆/CZTSe dual-absorber-like photovoltaic structure. The reported ETL-assisted and ETL-free device performances represent an idealized prediction under SCAPS-1D simulation conditions, because practical effects such as shunting, pinholes, interfacial inhomogeneity, and contact barriers were not explicitly considered. It is hoped that this work would extend the literature for Cs₂TiBr₆-based PSC with and without incorporating the ETL.

Data availability

All the data used in the work are already contained herein. There is no other data about this work to share.

Declaration of competing interest

The authors declare that there are no financial interests, commercial affiliations, or other potential conflicts of interest that could have influenced the objectivity of this research or the writing of this paper.

Funding

This work was supported by the UKRI Ayrton Fund: REACH-PSM – Resilient Renewable Energy Access through Community-Driven Holistic Development in Perovskite Solar Module Manufacturing.

References

- [1] G. M. Idroes, I. Hardi, M. H. Rahman, M. Afjal, T. R. Noviandy & R. Idroes, "The dynamic impact of non-renewable & renewable energy on carbon dioxide emissions & ecological footprint in Indonesia", *Carbon Research* **3** (2024) 35. <https://doi.org/10.1007/s44246-024-00117-0>.
- [2] P. R. Jubu, E. Danladi, H. F. Chahul, A. Aldayyat, Y. Yusof, K. M. Chahrour, P. I. Kyesmen, M. D. Tyonla, L. T. Abiem & F. K. Yam, "Photoanodic properties of In/ β -Ga₂O₃ nanostructures fabricated under hydrogen-reducing ambient by the vapour-phase growth method", *Optical Materials* **145** (2023) 114424. <https://doi.org/10.1016/j.optmat.2023.114424>.
- [3] P. I. Kyesmen, J. Simfukwe, P. R. Jubu, A. O. Adeola & M. Diala, "Structural properties & photoelectrocatalytic response of Mn-doped hematite photoanodes prepared via a modified electrodeposition approach", *ChemElectroChem* **11** (2024) e202400348. <https://doi.org/10.1002/celec.202400348>.
- [4] M. Ayoub & I. Dincer, "Experimental evaluation of photocatalytic & photoelectrochemical hydrogen fuel production with metal based catalysts, electrodes & coatings in a novel manner", *Fuel* **406** (2026) 136722. <https://doi.org/10.1016/j.fuel.2025.136722>.
- [5] K. Wang, J. Zheng, R. Yu & Z. Tan, "Recent progress on high efficiency perovskite/organic tandem solar cells", *Nanomaterials* **15** (2025) 745. <https://doi.org/10.3390/nano15100745>.
- [6] V. Krishnapressad, S. S. Parui & R. R. Babu, "Unveiling the potential of spray coated Cs₃Bi₂I₉ based perovskite solar cells: Numerical insights & experimental realization", *Materials Science & Engineering B* **323** (2026) 118684. <https://doi.org/10.1016/j.mseb.2025.118684>.
- [7] S. Zeng, A. Tanveer, X. Fu, Y. Gu & M. Irfan, "Modeling the influence of critical factors on the adoption of green energy technologies", *Renewable & Sustainable Energy Reviews* **168** (2022) 112817. <https://doi.org/10.1016/j.rser.2022.112817>.
- [8] R. A. Afre & D. Pugliese, "Perovskite solar cells: A review of the latest advances in materials, fabrication techniques & stability enhancement strategies", *Micromachines* **15** (2024) 192. <https://doi.org/10.3390/mi15020192>.
- [9] S. Gupta, J. Kaur, R. Basu, A. K. Sharma, R. Pandey & J. Madan, "Lead-free Cs₂TiBr₆ perovskite solar cells achieving high power conversion efficiency through device simulation", *Micro & Nanostructures* **196** (2024) 207991. <https://doi.org/10.1016/j.micrna.2024.207991>.
- [10] W. Lin, X. Chen, Z. Ji, W. Gao, N. Zhao, M. Li, D. Zhang, Y. Ling, J. Wu, K. Huang & J. Yu, "Optimization of Cs₂TiBr₆/CZTSe photoactive heterojunction perovskite solar cells with double hole transport layer by SCAPS-1D simulation", *Materials Today Communications* **46** (2025) 112841. <https://doi.org/10.1016/j.mtcomm.2025.112841>.
- [11] M. Chen, A. D. Carl, Y. Zong, R. L. Grimm, J. Gu, X.-C. Zeng & N. P. Padture, "Cesium titanium (IV) bromide thin films based stable lead-free perovskite solar cells", *Joule* **2** (2018) 558. <https://doi.org/10.1016/j.joule.2018.01.009>.
- [12] H. Karmaker, A. Siddique & B. K. Das, "Numerical investigation of lead-free Cs₂TiBr₆/CZTSe photoactive heterojunction perovskite solar cell with optimal selection of electron & hole transport layer through SCAPS-1D simulation", *Results in Optics* **13** (2023) 100571. <https://doi.org/10.1016/j.rso.2023.100571>.
- [13] M. K. Hossain, S. Islam, M. N. Sakib, M. S. Uddin, G. F. I. Toki, M. H. K. Rubel, J. Nasrin, S. H. Shahatha, M. R. Mohammad, A. A. Alothman, C. J. Raorane, R. Haldhar & H. Bencherif, "Exploring the optoelectronic & photovoltaic characteristics of lead-free Cs₂TiBr₆ double perovskite solar cells: A DFT & SCAPS-1D investigation", *Advanced Electronic Materials* **11** (2025) 2400348. <https://doi.org/10.1002/aelm.202400348>.
- [14] P. A. M. Mercy, K. & S. J. Wilson, "Development of environmentally friendly high-performance Cs₂TiBr₆/CZTSe photoactive heterojunction perovskite solar cell using numerical simulation", *Applied Surface Science Advances* **15** (2023) 100394. <https://doi.org/10.1016/j.apsadv.2023.100394>.
- [15] S. S. Urmi, M. A. K. Khan, T. T. Ferdous, D. Adinehloo, V. Perebeinos & M. A. Alim, "Cs₂TiI₆ (Cs₂TiI_xBr_{6-x}) halide perovskite solar cell & its point defect analysis", *Nanomaterials* **13** (2023) 2100. <https://doi.org/10.3390/nano13142100>.
- [16] J. Kaur, A. K. Sharma & R. Basu, "Numerical simulation & performance optimization of non-toxic Cs₂TiBr₆ single-halide perovskite solar cell by

- introducing interfacial defect layers", *Optical & Quantum Electronics* **57** (2025) 152. <https://doi.org/10.1007/s11082-024-08023-w>.
- [17] L. Salgado-Conrado, C. Álvarez-Macías & B. Reyes-Durán, "A review of simulation tools for thin-film solar cells", *Materials* **17** (2024) 5213. <https://doi.org/10.3390/ma17215213>.
- [18] P. R. Jubu, B. J. Akeredolu, S. J. Ikwee, K. O. Ighodalo, O. S. Obaseki, Z. S. Mbalah, S. K. Omotayo, Y. Yusof & M. Z. Pakhuruddin, "Performance optimization of perovskite solar cells using p-InGaAs as a hole transport layer: A numerical comparison with spiro-OMeTAD & HTL-free designs", *Next Energy* **11** (2026) 100510. <https://doi.org/10.1016/j.nxener.2025.100510>.
- [19] M. Aliaghayee, "An overview of numerical modeling, simulation & optimization methods toward the design of highly efficient planar perovskite solar cells", *Discover Electronics* **1** (2024) 35. <https://doi.org/10.1007/s44291-024-00026-x>.
- [20] S. M. Seyed-Talebi, M. Mahmoudi & C.-H. Lee, "A comprehensive study of CsSnI₃-based perovskite solar cells with different hole transporting layers & back contacts", *Micromachines* **14** (2023) 1562. <https://doi.org/10.3390/mi14081562>.
- [21] S. Chatterjee & A. J. Pal, "Introducing Cu₂O thin films as a hole-transport layer in efficient planar perovskite solar cell structures", *Journal of Physical Chemistry C* **120** (2016) 1428. <https://doi.org/10.1021/acs.jpcc.5b11540>.
- [22] A. Teyou Ngoupo, S. Ouédraogo, F. Zougmore & J. M. B. Ndjaka, "Numerical analysis of ultrathin Sb₂Se₃-based solar cells using SCAPS 1D", *Solar Energy* **194** (2021) 886. <https://doi.org/10.1016/j.cjph.2020.12.010>.
- [23] A. Benami, T. Ouslimane, L. Et-taya & A. Sohani, "Comparison of the effects of ZnO & TiO₂ on the performance of perovskite solar cells via SCAPS-1D software package", *Journal of Nano- & Electronic Physics* **14** (2022) 01033. [https://doi.org/10.21272/jnep.14\(1\).01033](https://doi.org/10.21272/jnep.14(1).01033).
- [24] D. Eli, M. Y. Onimisi, S. Garba, R. U. Ugbe, J. A. Owolabi, O. O. Ige, G. J. Ibeh & A. O. Muhammed, "Simulation & Optimization of Lead-Based Perovskite Solar Cells with Cuprous Oxide as a P-type Inorganic Layer," *Journal of the Nigerian Society of Physical Sciences* **1** (2019) 57. <https://doi.org/10.46481/jnsps.2019.13>.
- [25] I. T. Bello, Y. A. Odedunmoye, O. Adedokun, H. A. Shittu & A. O. Awodugba, "Numerical Simulation of Sandwiched Perovskite-Based Solar Cell Using Solar Cell Capacitance Simulator (SCAPS-1D)," *Journal of the Nigerian Society of Physical Sciences* **1** (2019) 57. <https://journal.nspss.org.ng/index.php/jnsps/article/view/11>.
- [26] E. Danladi, E. E. Oguzie & F. I. Ezema, "Highly efficient 25.562% Cs₂AgBiBr₆ double perovskite solar cell with copper barium tin sulfide & ZnO as charge transport channels: an intuition from a theoretical study using SCAPS-1D", *Journal of Photonics for Energy* **15** (2025) 024501. <https://doi.org/10.1117/1.JPE.15.024501>.
- [27] R. Kumar, S. Maity, D. K. Singh & P. K. Sahu, "Optimization of absorber layer Cs₂TiBr₆ dimension based on Portio Spider Algorithm for efficient lead-free perovskite solar cells", *Journal of Multiscale Modelling* **16** (2025) 2550010. <https://doi.org/10.1142/S1756973725500106>.
- [28] M. A. B. Siddique, N. Shahadath, M. Tarekuzzaman, M. Raihan Kabir, S. Ahmad, R. M. Khokan, M. Rasheduzzaman, S. M. G. Mostafa, M. J. Uddin & M. Z. Hasan, "Performance evaluation of Eu₂NiMnO₆-based lead-free perovskite solar cells: A SCAPS-1D study", *RSC Advances* **15** (2025) 35488. <https://doi.org/10.1039/d5ra05366h>.
- [29] M. Burgelman, P. Nollet & S. Degraeve, "Modelling polycrystalline semiconductor solar cells", *Thin Solid Films* **361** (2000) 527. [https://doi.org/10.1016/S0040-6090\(99\)00825-1](https://doi.org/10.1016/S0040-6090(99)00825-1).
- [30] J. Tauc, R. Grigorovici & A. Vancu, "Optical Properties & Electronic Structure of Amorphous Germanium", *Physica Status Solidi* **15** (1966) 627. <https://doi.org/10.1002/pssb.19660150224>.
- [31] A. Crovetto & O. Hansen, "What is the band alignment of Cu₂ZnSn(S,Se)₄ solar cells?", *Solar Energy Materials & Solar Cells* **169** (2017) 177. <https://doi.org/10.1016/j.solmat.2017.05.008>.
- [32] H. Dong, X. Yang, Y. Song, Z. Xu, Y. Liu, C. Han, J. Wu, Z. He & Q. Jiang, "Low-temperature processed cerium oxide electron transport layers for high-performance perovskite solar cells", *Journal of Materials Chemistry A* **11** (2023) 14521. <https://doi.org/10.1039/D3TA01564H>.
- [33] S. A. Moiz, "Optimization of Hole and Electron Transport Layer for Highly Efficient Lead-Free Cs₂TiBr₆-Based Perovskite Solar Cell", *Photonics* **9** (2022) 23. <https://doi.org/10.3390/photonics9010023>.
- [34] P. Singh & N. M. Ravindra, "Temperature dependence of solar cell performance—an analysis", *Solar Energy Materials & Solar Cells* **101** (2012) 36. <https://doi.org/10.1016/j.solmat.2012.02.019>.
- [35] V. Arjun, K. P. Muthukumaran, K. Ramachandran, A. Nithya & S. Karupuchamy, "Fabrication of efficient & stable planar perovskite solar cell using copper oxide as hole transport material", *Journal of Alloys & Compounds* **923** (2022) 166285. <https://doi.org/10.1016/j.jallcom.2022.166285>.
- [36] C. Zuo & L. Ding, "Solution-processed Cu₂O & CuO as hole transport materials for efficient perovskite solar cells", *Small* **11** (2015) 5528. <https://doi.org/10.1002/sml.201501330>.
- [37] X. Wang, L. Deng & L. Wang, "Cerium oxide standing out as an electron transport layer for efficient & stable perovskite solar cells processed at low temperature", *Journal of Materials Chemistry A* **5** (2017) 1706. <https://doi.org/10.1039/c6ta07541j>.
- [38] M. M. Haque, S. Mahjabin, S. Khan, M. S. Islam, M. A. K. Azad & M. M. Rahman, "Study on the interface defects of eco-friendly perovskite solar cells", *Solar Energy* **247** (2022) 96. <https://doi.org/10.1016/j.solener.2022.10.024>.
- [39] F. Liu, J. Zhu, J. Wei, Y. Li, M. Lv, S. Yang, B. Zhang, J. Yao & S. Dai, "Numerical simulation: Toward the design of high-efficiency planar perovskite solar cells", *Applied Physics Letters* **104** (2014) 253508. <https://doi.org/10.1063/1.4885367>.
- [40] M. K. Hossain, M. S. Uddin, G. F. I. Toki, M. K. A. Mohammed, R. Pandey, J. Madan, M. F. Rahman, M. R. Islam, S. Bhattarai, H. Bencherif, D. P. Samajdar, M. Amammi & D. K. Dwivedi, "Achieving above 24% efficiency with non-toxic CsSnI₃ perovskite solar cells by harnessing the potential of the absorber & charge transport layers", *RSC Advances* **13** (2023) 23514. <https://doi.org/10.1039/D3RA02910G>.
- [41] M. Grätzel, "Dye-sensitized solar cells", *Journal of Photochemistry & Photobiology C: Photochemistry Reviews* **4** (2003) 145. [https://doi.org/10.1016/S1389-5567\(03\)00026-1](https://doi.org/10.1016/S1389-5567(03)00026-1).
- [42] Y. Wu, X. Yang, H. Chen, K. Zhang, C. Qin, J. Liu, W. Peng, A. Islam, E. Bi & F. Ye, "Highly compact TiO₂ layer for efficient hole-blocking in perovskite solar cells", *Applied Physics Express* **7** (2014) 052301. <https://doi.org/10.7567/APEX.7.052301>.
- [43] H. B. Michaelson, "The work function of the elements and its periodicity", *Journal of Applied Physics* **48** (1977) 4729. <https://doi.org/10.1063/1.323539>.
- [44] N. Yadav & A. Khare, "Resolving interfacial challenges in perovskite solar cells: From defect control to energy band optimization", *Surfaces & Interfaces* **56** (2025) 105593. <https://doi.org/10.1016/j.surf.2024.105593>.
- [45] A. M. Cowley & S. M. Sze, "Surface states & barrier height of metal-semiconductor systems", *Journal of Applied Physics* **36** (1965) 3212. <https://doi.org/10.1063/1.1702952>.
- [46] R. T. Tun, "The physics & chemistry of the Schottky barrier height Free", *Applied Physics Reviews* **1** (2014) 011304. <https://doi.org/10.1063/1.4858400>.
- [47] D. Walter, J. Peng, K. Weber, K. R. Catchpole & T. P. White, "Performance limitations imposed by the TCO heterojunction in high efficiency perovskite solar cells", *Energy & Environmental Science* **15** (2022) 5202. <https://doi.org/10.1039/D2EE01742C>.
- [48] M. J. Heredia-Rios, L. Hernandez-Martinez, M. Linares-Aranda, M. Moreno-Moreno & J. F. Méndez, "Analysis of losses associated with series resistance (rs) in simple-structured c-si solar cells", *Energies* **17** (2024) 1520. <https://doi.org/10.3390/en17071520>.
- [49] M. A. Green, E. D. Dunlop, M. Yoshita, N. Kopidakis, K. Bothe, G. Siefer, X. Hao & J. Y. Jiang, "Solar cell efficiency tables (Version 64)", *Progress in Photovoltaics: Research & Applications* **32** (2024) 425. <https://doi.org/10.1002/pip.3831>.
- [50] M. A. B. Siddique, M. S. Parves, M. Tarekuzzaman, M. R. Kabir, M. S. M. Al-Saleem, J. Y. Al-Humaidi, M. Rasheduzzaman, M. M. Hossen, M. M. Rahman & M. Z. Hasan, "Exploring optoelectronic behavior & solar cell efficiency of double halide perovskites M₂KrCl₆ (M = Cs, Rb) through DFT & SCAPS-1D", *Langmuir* **41** (2025) 19797. <https://doi.org/10.1021/acs.langmuir.5c01639>.
- [51] F. Wang, Y. Gao, Z. Pang, L. Yang & J. Yang, "Insights into the role of the interface defects density & the bandgap of the back surface field for efficient p-type silicon heterojunction solar cells", *RSC Advances* **7** (2017) 26776. <https://doi.org/10.1039/C7RA04018K>.
- [52] Z. Xin, S. Duttgupta, M. Tang, Z. Qiu, B. Liao, & A. G. Aberle, "An

- improved methodology for extracting the interface defect density of passivated silicon solar cells", *IEEE Journal of Photovoltaics* **6** (2016) 1080. <https://doi.org/10.1109/JPHOTOV.2016.2576685>.
- [53] T. Ouslimane, L. Et-taya, L. Elmaimouni & A. Benami, "Impact of absorber layer thickness, defect density & operating temperature on the performance of MAPbI₃ solar cells based on ZnO electron transporting material", *Heliyon* **7** (2021) e06379. <https://doi.org/10.1016/j.heliyon.2021.e06379>.
- [54] T. S. Sherkar, C. Mombona, L. Gil-Escrig, J. Ávila, M. Sessolo, H. J. Bolink & L. J. A. Koster, "Recombination in perovskite solar cells: Significance of grain boundaries, interface traps & defect ions", *ACS Energy Letters* **2** (2017) 1214. <https://doi.org/10.1021/acsenergylett.7b00236>.
- [55] Z. Ni, S. Xu, D. P. McMeekin, S. M. Wood, H. A. Mohd Yusof, X. Wang et al., "Resolving spatial & energetic distributions of trap states in metal halide perovskite solar cells", *Science* **367** (2020) 1352. <https://doi.org/10.1126/science.aba0893>.
- [56] E. Danladi, E. E. Oguzie & F. I. Ezema, "Highly efficient 25.562% Cs₂AgBiBr₆ double perovskite solar cell with copper barium tin sulfide & ZnO as charge transport channels: an intuition from a theoretical study using SCAPS-1D", *Journal of Photonics for Energy* **15** (2025) 024501. <https://doi.org/10.1117/1.JPE.15.024501>.
- [57] S. Heo, G. Seo, Y. Lee, D. Lee, M. Seol, J. Lee, J.-B. Park, K. Kim, D.-J. Yun, Y. S. Kim, J. K. Shin, T. K. Ahn & M. K. Nazeruddin, "Deep level trapped defect analysis in CH₃NH₃PbI₃ perovskite solar cells by deep level transient spectroscopy", *Energy & Environmental Science* **10** (2017) 1128. <https://doi.org/10.1039/c7ee00303j>.
- [58] P. K. Patel, "Device simulation of highly efficient eco-friendly CH₃NH₃SnI₃ perovskite solar cell", *Scientific Reports* **11** (2021) 3082. <https://doi.org/10.1038/s41598-021-82817-w>.
- [59] J. Siekmann, S. Ravishanker & T. Kirchartz, "Apparent defect densities in halide perovskite thin films & single crystals", *ACS Energy Letters* **6** (2021) 3244. <https://doi.org/10.1021/acsenergylett.1c01449>.
- [60] G. F. Brown & J. Wu, "Third generation photovoltaics", *Laser & Photonics Reviews* **3** (2009) 394. <https://doi.org/10.1002/lpor.200810039>.
- [61] S. Rühle, "Tabulated values of the Shockley–Queisser limit for single junction solar cells", *Solar Energy* **130** (2016) 139. <https://doi.org/10.1016/j.solener.2016.02.015>.
- [62] M. Rehan, H. Jeon, Y. Cho, A. Cho, K. Kim, J.-S. Cho, J. H. Yun, S. Ahn, J. Gwak, D. Shin, "Fabrication & characterization of Cu₂ZnSnSe₄ thin-film solar cells using a single-stage co-evaporation method: Effects of film growth temperatures on device performances", *Energies* **13** (2020) 1316. <https://doi.org/10.3390/en13061316>.
- [63] Y. Liu, X. Xu, K. Liu & H. Liu, "Synthesis of Cu₂ZnSnSe₄ thin-film solar cells from nanoparticles by a non-vacuum mechanical ball milling & rapid thermal processing", *Micro & Nano Letters* **15** (2020) 887. <https://doi.org/10.1049/mnl.2019.0788>.
- [64] F.-I. Lai, J.-F. Yang, Y.-L. Wei & S.-Y. Kuo, "High quality sustainable Cu₂ZnSnSe₄ (CZTSe) absorber layers in highly efficient CZTSe solar cells", *Green Chemistry* **19** (2017) 795. <https://doi.org/10.1039/C6GC02300B>.
- [65] R. Sen & M. Yadav, "Efficient design & fabrication of Cs₂TiBr₆/CZTSe photoactive heterojunction HTL-free solar cells", *Journal of Electronic Materials* **53** (2024) 1975. <https://doi.org/10.1007/s11664-024-10929-w>.
- [66] M. M. Alam, R. K. S. Durjoy, M. A. Patwary, A. A. Shafin, M. S. Su'ait, M. Shahiduzzaman, M. Akhtaruzzaman, M. Mottakin, "Enhancing the performance of Cs₂TiBr₆ lead-free perovskite solar cells: a simulation study on the impact of electron and hole transport layers", *Langmuir* **41** (2025) 6987. <https://doi.org/10.1021/acs.langmuir.4c05265>.
- [67] J. Pascual, I. Kosta, T. Ngo, A. Chuvinil, G. Cabanero, H. J. Grande, E. M. Barea, I. Mora-Seró, J. L. Delgado & R. Tena-Zaera, "Electron transport layer-free solar cells based on perovskite–fullerene blend films with enhanced performance & stability", *ChemSusChem* **9** (2016) 2679. <https://doi.org/10.1002/cssc.201600940>.
- [68] M. K. Omar, M. Rashid & M. Z. Pakhuruddin, "Simulation of homo-junction p-i-n indium nitride solar cells under high sunlight concentration", *Physica Scripta* **100** (2025) 065527. <https://doi.org/10.1088/1402-4896/add392>.
- [69] M. Chegaar, A. Hamzaoui, A. Namoda, P. Petit, M. Aillerie & A. Herguth, "Effect of illumination intensity on solar cells parameters", *Energy Procedia* **36** (2013) 722. <https://doi.org/10.1016/j.egypro.2013.07.084>.
- [70] P. Pérez-Higueras, E. Muñoz, G. Almonacid & P. G. Vidal, "High concentrator photovoltaics efficiencies: Present status & forecast", *Renewable & Sustainable Energy Reviews* **15** (2011) 1810. <https://doi.org/10.1016/j.rser.2010.11.046>.
- [71] M. Wolf & H. Rauschenbach, "Series resistance effects on solar cell measurements", *Advanced Energy Conversion* **3** (1963) 455. [https://doi.org/10.1016/0365-1789\(63\)90063-8](https://doi.org/10.1016/0365-1789(63)90063-8).
- [72] H.-Y. Ryu, G.-H. Ryu, Y.-H. Choi & B. Ma, "Modeling & simulation of efficiency droop in GaN-based blue light-emitting diodes incorporating the effect of reduced active volume of InGaN quantum wells", *Current Applied Physics* **17** (2017) 1298. <https://doi.org/10.1016/j.cap.2017.06.014>.
- [73] A. Najim, L. Moulaoui, A. Bakour, O. Bajjou, K. Rahmani, "High-efficiency numerical modeling of rGO/P3HT solar cells using SCAPS-1D", *Journal of Optics* **55** (2026) 1048. <https://doi.org/10.1007/s12596-024-02112-5>.
- [74] L. Huang, X. Sun, C. Li, R. Xu, J. Xu, Y. Du, Y. Wu, J. Ni, H. Cai, J. Li, Z. Hu & J. Zhang, "Electron transport layer-free planar perovskite solar cells: Further performance enhancement perspective from device simulation", *Solar Energy Materials & Solar Cells* **157** (2016) 1038. <https://doi.org/10.1016/j.solmat.2016.08.025>.
- [75] W. Hui, X. Kang, B. Wang, D. Li, Z. Su, Y. Bao, L. Gu, B. Zhang, X. Gao, L. Song & W. Huang, "Stable electron-transport-layer-free perovskite solar cells with over 22% power conversion efficiency", *Nano Letters* **23** (2023) 2195. <https://doi.org/10.1021/acs.nanolett.2c04720>.
- [76] H. Pourfarzad, M. Saremi & R. Badrnezhad, "Study of performance & stability of hole transport layer-free perovskite solar cells with modified electron transport layer", *Journal of Materials Science: Materials in Electronics* **32** (2021) 17602. <https://doi.org/10.1007/s10854-021-06293-8>.
- [77] C. Huang, P. Lin, N. Fu, C. Liu, B. Xu, K. Sun, D. Wang, X. Zeng & S. Ke, "Facile fabrication of highly efficient ETL-free perovskite solar cells with 20% efficiency by defect passivation & interface engineering", *Chemical Communications* **55** (2019) 2777. <https://doi.org/10.1039/C9CC00312F>.
- [78] J. F. Liao, W. Q. Wu, Y. Jiang, J. Zhong, L. Wang & D. B. Kuang, "Understanding of carrier dynamics, heterojunction merits & device physics: Towards designing efficient carrier transport layer-free perovskite solar cells", *Chemical Society Reviews* **49** (2020) 354. <https://doi.org/10.1039/C8CS01012A>.
- [79] M. Gloeckler, A. L. Fahrenbruch & J. R. Sites, *Numerical modeling of CIGS & CdTe solar cells: Setting the baseline*, Proceedings of the 3rd World Conference on Photovoltaic Energy Conversion, Osaka, Japan, 2003, pp. 491-494, <https://ieeexplore.ieee.org/document/1305328/authors#authors>.
- [80] P. R. Jubu, M. K. Omar, S. K. Omotayo & M. Z. Pakhuruddin, "Numerical simulation on electrical characteristics of high efficiency PPN homojunction InGaN photovoltaic solar cell", *Next Materials* **11** (2026) 101597. <https://doi.org/10.1016/j.nxmate.2026.101597>.
- [81] M. Saadat & S. Bameri, "Comprehensive analysis of transport layers & interface defects in MAPbI₃ based PSCs for enhanced efficiency", *Discover Applied Sciences* **7** (2025) 440. <https://doi.org/10.1007/s42452-025-06948-9>.
- [82] S. R. Fahima, M. S. Sarker, M. I. Piya, J. A. Bhuiyan, H. Mamur & M. R. A. Bhuiyan, "Simulation, optimization & machine learning strategies for CH₃NH₃PbBr₃ perovskite solar cells", *Next Energy* **10** (2026) 100491. <https://doi.org/10.1016/j.nxener.2025.100491>.
- [83] P. Subudhi & A. R. Narasimhan, "Design & simulation of PEA_{0.15}FA_{0.75}MA_{0.1}SnI₂Br based quasi-2D/3D tin perovskite solar cells with different charge transport layers for efficiency enhancement", *Scientific Reports* **16** (2026) 11220. <https://doi.org/10.1038/s41598-026-54942-x>.
- [84] M. A. Rahman & M. J. Alam, "Optimization of lead-free perovskite solar cell architecture using machine learning & numerical simulations", *Advanced Theory & Simulations* **9** (2026) e01590. <https://doi.org/10.1002/adts.202501590>.
- [85] B. C. Biswas, A. I. Shimul, I. Paul, "Investigating the optoelectronic properties & photovoltaic performance of Na₂AuGaBr₆ based double perovskite solar cells via numerical simulation & AI techniques", *Scientific Reports* **16** (2026) 11218. <https://doi.org/10.1038/s41598-026-41519-x>.