

Numerical Optimization of Cd-Free CZTSe Kesterite Solar Cells with Tunable Zn(O,S) Buffer Layers Using Silvaco ATLAS

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Article Info:

DOI: -10.22399/ijcesen.5455

Received : 27 November 2025

Revised : 25 January 2026

Accepted : 07 March 2026

Keywords

CZTSe kesterite
Zn(O,S) buffer layer
Silvaco ATLAS
Cd-free solar cells
Device optimization

Abstract:

Conventional $\text{Cu}_2\text{ZnSnSe}_4$ (CZTSe) kesterite solar cells commonly employ toxic CdS buffer layers that introduce parasitic blue-light absorption, cadmium-related environmental hazards, and potentially unfavorable conduction-band offsets (CBOs) that contribute to the open-circuit-voltage deficit. This study numerically optimizes a fully Cd-free glass/Mo/p-CZTSe/n-Zn(O_xS_{1-x})/n-ZnO/ITO architecture using Silvaco ATLAS TCAD. The model solves the self-consistent Poisson, drift-diffusion, and carrier-continuity equations with Shockley-Read-Hall (SRH), radiative, and Auger recombination under AM1.5G illumination (100 mW cm⁻², 300 K). A compositional sweep of Zn(O_xS_{1-x}) ($x = 0$ to 1) identifies Zn(O_{0.4}S_{0.6}) as the optimum buffer, yielding $\eta = 12.79\%$, $J_{sc} = 39.47$ mA cm⁻², $V_{oc} = 461.66$ mV, and FF = 70.24% for the baseline dimensions. Subsequent optimization of the CZTSe thickness (4 μm), Zn(O,S) thickness (0.05 μm), ZnO thickness (0.06 μm), and CZTSe acceptor density ($N_A = 1.4 \times 10^{15}$ cm⁻³) increases the simulated performance to $\eta = 14.13\%$, $J_{sc} = 41.20$ mA cm⁻², $V_{oc} = 483.08$ mV, and FF = 71.02%. Simulations from 240 to 350 K show monotonic degradation of V_{oc} and η with temperature, consistent with SRH-dominated bulk recombination. The results provide a physically grounded, simulation-guided basis for Cd-free CZTSe device engineering and require experimental validation.

1. Introduction

Photovoltaic energy conversion is a key component of the transition toward sustainable electricity because it directly converts an abundant solar resource into electrical power. Within this context, thin-film photovoltaic (PV) technologies are attractive because they reduce active-material consumption and are compatible with scalable fabrication [1,2]. CdTe and Cu(In,Ga)Se₂ (CIGS) devices have achieved power conversion efficiencies in the 22 to 23% range owing to mature processing routes and favorable optoelectronic properties [1,3]. Their reliance on scarce or hazardous constituents, however, raises concerns regarding resource availability, environmental regulation, and long-term supply. These limitations have intensified interest in kesterite

$\text{Cu}_2\text{ZnSn}(\text{S,Se})_4$ absorbers, which are composed of abundant elements, exhibit absorption coefficients above 10⁴ cm⁻¹ [2], and offer a tunable direct band gap of approximately 1.0 to 1.5 eV [4,5].

The selenide-rich kesterite $\text{Cu}_2\text{ZnSnSe}_4$ (CZTSe) is particularly attractive for single-junction thin-film cells because its band gap of approximately 1.0 to 1.1 eV supports broad solar-spectrum absorption, while optimized experimental and simulated devices commonly exhibit efficiencies in the 10 to 13% range [6]. Nevertheless, CZTSe cells remain limited by complex bulk-defect chemistry, cation-anion site disorder, and non-ideal absorber/buffer band alignment, which contribute to the characteristic open-circuit-voltage deficit and fill-factor losses [7,8]. A conventional device generally consists of a Mo-coated substrate, a p-type CZTSe absorber, an n-type CdS buffer deposited by

chemical bath deposition, and a ZnO-based transparent front contact [9,10]. In a related Silvaco ATLAS study, simultaneous optimization of layer thickness and doping concentration increased the simulated efficiency of a ZnO/CdS/CZTSSe cell from 12.73% to 18.75%, confirming that optical absorption, junction electrostatics, and recombination must be considered together [9].

Although CdS forms the p-n heterojunction and protects the absorber surface during deposition, it also introduces environmental and device-performance constraints [11,12]. Cadmium-related toxicity requires careful control during manufacturing and end-of-life management [13], while the approximately 2.4 eV CdS band gap causes parasitic short-wavelength absorption that reduces the useful photocurrent [7,10]. Moreover, an unfavorable conduction-band offset at the CZTSe/CdS interface can intensify interface recombination and suppress the open-circuit voltage [7,8]. These limitations have motivated the investigation of Cd-free alternatives, including ZnO, ZnS, ZnSe, Zn(O,S), ZnSnO, TiO₂, and multilayer buffer configurations [10,14]. The improvement obtained with thin ZnO, ZnSe, and ZnS buffers in CdTe simulations further supports the optical and environmental rationale for wide-band-gap zinc-based buffers, although their optimum band alignment cannot be transferred directly to CZTSe because it is absorber-specific [7].

Among the proposed alternatives, zinc oxysulfide Zn(O_xSi_{1-x}) provides direct control of the heterojunction energetics because both its band gap and electron affinity vary with the oxygen-to-sulfur ratio. Using the convention $\Delta E_c = E_{C,buffer} - E_{C,absorber}$, composition tuning can shift the interface from a transport-blocking positive spike, through near-flat alignment, to a recombination-promoting negative cliff [15,16]. Experimental CZTSSe/Zn(O,S) heterojunctions deposited by high-vapor-transport deposition achieved efficiencies of 6.87 to 9.82%, showing that intermediate oxygen contents can avoid the two unfavorable alignment extremes [17,18]. ZnS(O,OH) double buffers have also improved V_{oc} relative to CdS references, with performance strongly dependent on chemical-bath composition [19]. These findings demonstrate that Zn(O,S) composition and thickness must be optimized simultaneously rather than treated as independent parameters.

Recent numerical studies across thin-film and emerging photovoltaic architectures reinforce this coupled-optimization approach [20]. An MgZnO/i-CIGS/CIGS structure reached its best simulated

response with a 4 μm absorber and a 0.05 μm MgZnO layer at 290 K [21], whereas organic cells exhibited architecture-dependent optimum active-layer thicknesses [22]. Composition engineering in Cd_{1-x}Zn_xTe produced a trade-off between improved V_{oc} and preserved J_{sc} [23], and CIGS/ASnI₂Br and CsSnI₃ investigations identified energy-level alignment, absorber thickness, doping, defect density, parasitic resistances, and temperature as interdependent performance variables [24-27]. Alloy-fraction sweeps in BGaN modeling provide an additional methodological precedent for composition-dependent band-gap analysis, although photodetector figures of merit are not directly comparable with photovoltaic efficiency [28].

Within the literature considered here, a unified Silvaco ATLAS analysis that combines Zn(O,S) composition, absorber/buffer/window thicknesses, CZTSe acceptor concentration, and operating temperature for a single-junction CZTSe device remains insufficiently developed. The present study therefore investigates a fully Cd-free glass/Mo/p-CZTSe/n-Zn(O_xSi_{1-x})/n-ZnO/ITO architecture under AM1.5G illumination. The analysis proceeds through four coordinated stages: Zn(O,S) compositional optimization to establish a favorable conduction-band offset, CZTSe absorber-thickness optimization, buffer- and ZnO-window-thickness optimization, and absorber-doping optimization. The resulting baseline and optimized devices are compared through J_{sc} , V_{oc} , fill factor, power conversion efficiency, and temperature-dependent current-voltage behavior, providing a simulation-guided framework for experimental Cd-free CZTSe device engineering.

2. Material and Methods

2.1 Device Architecture and Baseline Parameters

The simulated device is a planar single-junction CZTSe thin-film solar cell with the layer sequence: glass / Mo (0.5 μm) / p-CZTSe / n-Zn(O_xSi_{1-x}) / n-ZnO / ITO, illuminated from the front (ITO/ZnO side). The molybdenum back contact provides an ohmic junction to the p-type CZTSe absorber; the ZnO window (baseline: 0.2 μm) ensures lateral carrier collection and optical transparency; and the Zn(O_xSi_{1-x}) buffer (baseline: 0.05 μm) forms the primary heterojunction with composition x controlling the CBO. The layer stack and complete baseline electrical parameters are shown in Figure 1 and Table 1, respectively, and are cross-validated against CZTSe, CdTe, and CIGS literature [1,2,29].

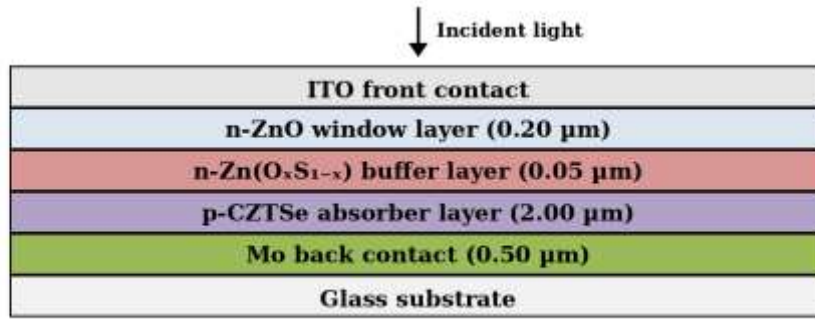


Figure 1. Schematic layer structure of the baseline glass/Mo/CZTSe/Zn(O,S)/ZnO/ITO solar cell. Illumination is incident through the ITO front contact.

Table 1. Baseline electrical input parameters for the CZTSe/Zn(O,S)/ZnO solar cell [1,2,29].

Parameter	n-ZnO (window)	n-Zn(O,S) (buffer)	p-CZTSe (absorber)
E_g (eV)	3.30	2.72 to 3.60 (variable)	1.04
χ (eV)	4.50	3.38 to 4.78 (variable)	4.10
ϵ_r (-)	9	10	10
N_C (cm ⁻³)	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}
N_V (cm ⁻³)	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Doping (cm ⁻³)	$N_D = 10^{19}$	$N_D = 10^{17}$	$N_A = 10^{15}$
μ_n (cm ² V ⁻¹ s ⁻¹)	100	100	100
μ_p (cm ² V ⁻¹ s ⁻¹)	25	25	25
Defect type	Donor	Acceptor	Donor
N_t (cm ⁻³)	10^{17}	5×10^{16}	10^{14}

Note. Baseline electrical parameters. Variable E_g and χ for Zn(O,S) are defined by the piecewise compositional model (see Table 2).

The Zn(O,S) buffer band edges are defined at discrete compositions x according to Table 2, consistent with reported Zn(O,S) optical band gaps and electron affinities for CBD and HVTD films [30,31]. These values define the CBO at the CZTSe/Zn(O,S) interface and the VBO at the Zn(O,S)/ZnO junction, enabling explicit mapping between composition x and band alignment regimes (cliff-like, flat, or spike-like) [30-34].

Table 2. Composition-dependent E_g and χ of Zn(O_xS_{1-x}) buffer layer [18].

Composition x	E_g (eV)	χ (eV)
0.0 (pure ZnS)	3.60	3.38
0.2	3.04	3.88
0.4	2.72	4.08
0.6	2.64	4.28
0.8	2.80	4.48
1.0 (pure ZnO)	3.20	4.78

2.2 Silvaco ATLAS Transport Equations

The device physics is solved using Silvaco ATLAS, which numerically integrates the coupled Poisson equation and electron/hole continuity equations within the drift-diffusion formalism [35]. The electrostatic potential $\phi(x)$ is determined from Poisson's equation:

$$\nabla \cdot (\epsilon_r \epsilon_0 \nabla \phi) = -q(p - n + N_D^+ - N_A^- + N_t) \quad (1)$$

where ϵ_r is the position-dependent relative permittivity, ϵ_0 the vacuum permittivity, q the elementary charge, n and p the electron and hole densities, N_D^+ and N_A^- the ionized donor and acceptor concentrations, and N_t the net charged trap density. Carrier dynamics are governed by the time-dependent continuity equations:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot J_n + G_n - R_n \quad (2)$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot J_p + G_p - R_p \quad (3)$$

where J_n and J_p are the electron and hole current densities, $G_{n,p}$ the optical generation rates, and $R_{n,p}$ the total recombination rates. Within the drift-diffusion framework, the current densities in one spatial dimension are:

$$J_n = q\mu_n nE + qD_n \frac{\partial n}{\partial x} \quad (4)$$

$$J_p = q\mu_p pE - qD_p \frac{\partial p}{\partial x} \quad (5)$$

where $E = -\partial\phi/\partial x$ is the electric field, $\mu_{n,p}$ the carrier mobilities, and $D_{n,p}$ the diffusion coefficients related through the Einstein relation. Equations (1)-(5) are solved self-consistently, iterating on ϕ , n , p , and J until numerical convergence under specified bias and illumination.

2.3 Recombination Models

Shockley-Read-Hall (SRH) recombination is modeled with mid-gap traps in each layer using the defect densities N_t from Table 1. The SRH recombination rate is:

$$R_{n,p} = \frac{\sigma_n \sigma_p v_{th} N_t (n p - n_i^2)}{\sigma_n [n + n_i \exp(\frac{E_t - E_i}{kT})] + \sigma_p [p + n_i \exp(\frac{E_t - E_i}{kT})]} \quad (6)$$

where n_i is the intrinsic carrier density, v_{th} the thermal velocity, $\sigma_{n,p}$ the carrier capture cross-sections, E_i the intrinsic Fermi level, and E_t the trap energy level. SRH recombination is the dominant loss mechanism in kesterite absorbers, governing V_{oc} deficits and FF degradation at practical defect densities [36]. Radiative and Auger recombination are also activated in all layers, but their contribution is secondary to SRH at polycrystalline CZTSe defect densities.

2.4 Boundary and Illumination Conditions

The rear Mo contact is implemented as an ohmic contact to p-CZTSe, with its work function set to eliminate any hole-extraction barrier. The front ITO/ZnO contact is likewise ohmic, with N_D (ZnO) = 10^{19} cm^{-3} ensuring negligible contact resistance. All simulations are performed under AM1.5G illumination at $P_{in} = 100 \text{ mW cm}^{-2}$ and $T = 300 \text{ K}$ unless otherwise stated.

2.5 Compositional Model for $\text{Zn}(\text{O}_x\text{S}_{1-x})$

The $\text{Zn}(\text{O},\text{S})$ buffer is modeled as $\text{Zn}(\text{O}_x\text{S}_{1-x})$ using piecewise-linear interpolation between the discrete data points in Table 2 for $E_g(x)$ and $\chi(x)$. This mapping captures the non-monotonic variation in band gap across the ZnS-ZnO compositional range [30,31], transitioning from wide-gap ZnS (3.6 eV, $\chi = 3.38 \text{ eV}$) to ZnO (3.2 eV, $\chi = 4.78 \text{ eV}$) via the minimum at $x = 0.6$ (2.64 eV).

3. Results and Discussions

3.1 Effect of $\text{Zn}(\text{O},\text{S})$ Composition and Band Alignment on Device Performance

A systematic sweep of the $\text{Zn}(\text{O}_x\text{S}_{1-x})$ composition x from 0 to 1 reveals a pronounced, non-monotonic dependence of all device metrics on buffer-layer band alignment, as summarized in Table 3 and illustrated in Figure 2. The response demonstrates that composition acts primarily through interfacial energetics and carrier selectivity rather than through a simple monotonic change in optical transparency.

Table 3. Device performance metrics as a function of $\text{Zn}(\text{O}_x\text{S}_{1-x})$ composition x (baseline structural dimensions).

x	Composition	$J_{sc} \text{ (mA cm}^{-2}\text{)}$	$V_{oc} \text{ (mV)}$	FF (%)	$\eta \text{ (%)}$
0.0	Pure ZnS	2.08	750.64	21.69	0.34
0.2	$\text{Zn}(\text{O}_{0.2}\text{S}_{0.8})$	39.30	472.56	51.90	9.63
0.4	$\text{Zn}(\text{O}_{0.4}\text{S}_{0.6})$	39.47	461.66	70.24	12.79
0.6	$\text{Zn}(\text{O}_{0.6}\text{S}_{0.4})$	39.76	462.82	69.09	12.71
0.8	$\text{Zn}(\text{O}_{0.8}\text{S}_{0.2})$	38.29	466.96	60.27	10.77
1.0	Pure ZnO	33.18	559.74	19.48	3.61

At $x = 0$ (pure ZnS), the low buffer electron affinity ($\chi = 3.38 \text{ eV}$) places the ZnS conduction-band minimum substantially above that of CZTSe, producing a large positive CBO (strong spike regime). This barrier impedes electron extraction across the heterojunction and suppresses minority-carrier collection. Despite a nominally high $V_{oc} = 750.64 \text{ mV}$, a value caused by the large junction built-in potential when meaningful photocurrent is absent, J_{sc} collapses to 2.08 mA cm^{-2} and FF to 21.69%, yielding $\eta = 0.34\%$. The result illustrates why V_{oc} cannot be interpreted independently of the generated current and the shape of the J-V curve.

As the oxygen content increases to $x = 0.2$, the rising electron affinity shifts the $\text{Zn}(\text{O},\text{S})$ conduction-band minimum toward that of CZTSe and substantially reduces the excessive positive spike. J_{sc} rises to 39.30 mA cm^{-2} and η to 9.63%, while FF improves to 51.90%, confirming that partial relief of the extraction barrier enables carrier collection. At $x = 0.4$, a near-neutral to slightly

spike-like CBO is achieved ($\Delta E_c \approx 0$ to $+0.05 \text{ eV}$), representing the optimum trade-off: $J_{sc} = 39.47 \text{ mA cm}^{-2}$, $V_{oc} = 461.66 \text{ mV}$, FF = 70.24%, and $\eta = 12.79\%$. This configuration suppresses interface recombination without imposing a substantial electron-transport barrier, explaining the pronounced FF improvement relative to lower x values [17,18].

For x values of 0.6 and above, the continued increase in χ shifts the buffer conduction band below that of CZTSe and produces an increasingly negative, cliff-like CBO. Although a shallow cliff can still permit electron extraction, a deeper cliff enhances interfacial recombination and progressively degrades FF and J_{sc} . At $x = 1$ (pure ZnO), FF collapses to 19.48% and J_{sc} falls to 33.18 mA cm^{-2} , yielding $\eta = 3.61\%$ despite V_{oc} recovering modestly to 559.74 mV. This behavior is consistent with experimental reports on $\text{Zn}(\text{O},\text{S})$ /kesterite heterojunctions in which excessive oxygen content reduces FF and

photocurrent while providing only marginal V_{oc} gains [17,18]. The optimum composition is therefore confirmed as $x = 0.4$ ($Zn(O_{0.4}S_{0.6})$), and the corresponding baseline J-V characteristic is shown in Figure 3. Comparison with the CdTe buffer-layer analysis in [7] reinforces that a wide band gap and the absence of cadmium do not by themselves guarantee efficient extraction. In that different absorber system, ZnS and ZnSe outperformed ZnO after thickness optimization; the ranking cannot be transferred directly to CZTSe because the band edges and interface defects differ, but both studies show that the buffer controls optical transmission and heterojunction transport simultaneously. Here, the larger V_{oc} values at $x = 0$ and $x = 1$ coincide with severe J_{sc} and FF losses, so the maximum PCE occurs at the intermediate composition that best balances recombination suppression and electron collection. A related composition-performance trade-off was obtained for $Cd_{1-x}Zn_xTe$ absorbers, where Zn incorporation improved voltage-related properties while an optimum composition was required to preserve photocurrent [23]. Composition-dependent bandgap and spectral-response changes were also demonstrated in B GaN simulations [28]; however, the device contacts and target metrics of that photodetector differ fundamentally from the present solar cell. These cross-system comparisons support the compositional-sweep methodology, but not transfer of the numerical optimum. Composition control should therefore precede thickness and doping optimization.

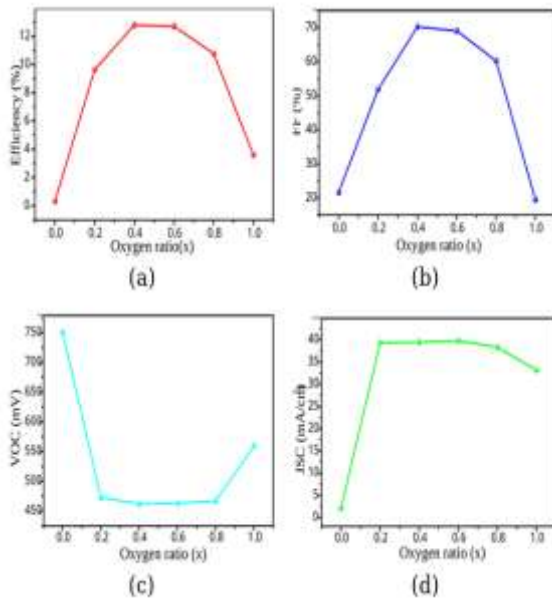


Figure 2. Effect of Zn(O,S) composition x on device performance: (a) Power conversion efficiency η , (b) Fill factor FF, (c) Open-circuit voltage V_{oc} , (d) Short-circuit current density J_{sc} .

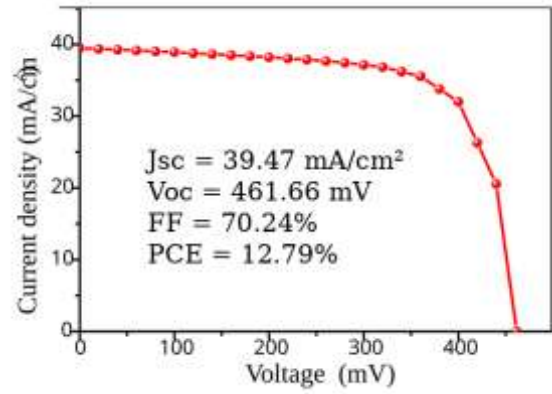


Figure 3. Current density-voltage (J-V) characteristic of the baseline CZTSe/Zn(O_{0.4}S_{0.6})/ZnO cell

3.2 Optimization of CZTSe Absorber Thickness

With Zn(O_{0.4}S_{0.6}) established as the optimum buffer, the CZTSe absorber thickness w_{CZTSe} is swept from 1 to 10 μm . As shown in Figure 4, η increases from $\approx 11.5\%$ at 1 μm to a plateau of $\approx 13.5\%$ at $\approx 4 \mu\text{m}$, followed by only marginal improvement and slight degradation for thicker absorbers. J_{sc} rises from $\approx 35 \text{ mA cm}^{-2}$ at 1 μm and saturates near $\approx 41 \text{ mA cm}^{-2}$ beyond 4 μm because of the increasing optical absorption volume. V_{oc} similarly stabilizes near $\approx 480 \text{ mV}$ beyond 4 μm , whereas FF improves from $\approx 30\%$ at 1 μm to $\approx 70\%$ for w_{CZTSe} values of 3 μm and above.

For w_{CZTSe} below 3 μm , incomplete spectral absorption limits J_{sc} and η ; for w_{CZTSe} above approximately 4 to 5 μm , photogenerated carriers created beyond the effective collection length are increasingly likely to recombine before reaching the junction, yielding diminishing returns in J_{sc} and FF. This general absorption-collection trade-off has also been observed in a different InGaP/GaAs dual-junction architecture [37], although its material system and optimum thickness are not directly transferable to the present CZTSe device. An absorber thickness of 4 μm therefore represents the practical optimum and is adopted as the fixed value for all subsequent optimizations. A comparable saturation mechanism was reported for a CdS-buffered CZTSe single-junction cell: light harvesting improved with thickness, but PCE decreased after the 2.5 μm optimum because the additional absorber increased bulk series resistance and generated carriers outside the effective collection range [9]. The non-universality of the optimum is also evident across the newly considered studies: MgZnO/CIGS optimization selected a 4 μm CIGS absorber [21]; inverted and conventional organic cells peaked at 220 and 240 nm, respectively [22]; and two lead-free CsSnI₃ architectures reported absorber optima of 600 nm

[25] and 300 nm [27]. These numerical values differ because absorption coefficients, mobilities, defect densities, interfaces, and collection lengths are system-specific. The difference between the 2.5 μm optimum in [9] and the present 4 μm value therefore confirms that optimum thickness is not a universal material constant; it depends on the buffer, defect density, transport parameters, and recombination assumptions used in the device model.

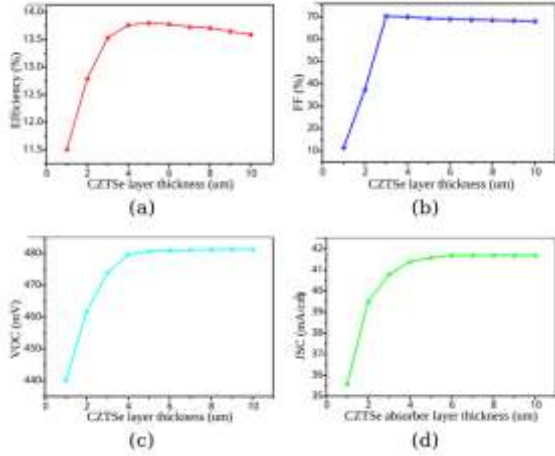


Figure 4. Device performance parameters as a function of CZTSe absorber thickness: (a) η , (b) FF, (c) V_{oc} , (d) J_{sc} . Optimum at $w_{CZTSe} = 4 \mu\text{m}$.

3.3 Optimization of Buffer and Window Layer Thicknesses

3.3.1 Zn(O,S) Buffer Thickness

The Zn(O_{0.4}S_{0.6}) buffer thickness w_{buf} is varied from ≈ 0.02 to 0.2 μm with the 4 μm CZTSe absorber fixed. Figure 5 summarizes the resulting trends.

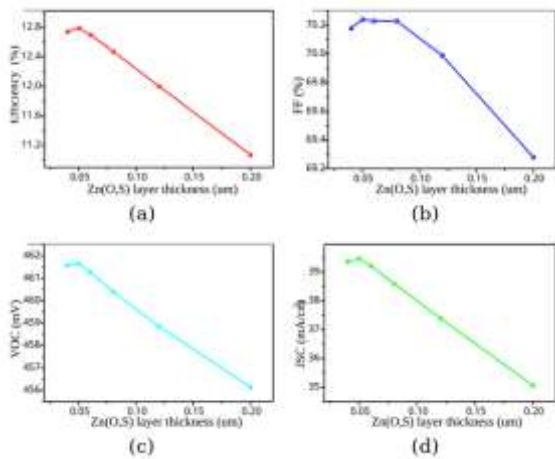


Figure 5. Device performance parameters as a function of Zn(O_{0.4}S_{0.6}) buffer layer thickness: (a) η , (b) FF, (c) V_{oc} , (d) J_{sc} .

Efficiency decreases progressively from $\approx 12.8\%$ at $w_{buf} \approx 0.02 \mu\text{m}$ to $\approx 11.2\%$ at 0.2 μm , accompanied by a decrease in J_{sc} from ≈ 39.5 to $\approx 35.5 \text{ mA cm}^{-2}$ and a drop in V_{oc} from ≈ 462 to $\approx 456 \text{ mV}$. FF remains stable near 70.2% for w_{buf} in the range 0.02

to 0.08 μm and then declines for thicker buffers because of rising transport resistance and the greater probability of recombination within the buffer volume. A related CIGS simulation likewise reported buffer-thickness-dependent transport losses [38], although its numerical optimum is not directly transferable to the present CZTSe/Zn(O,S) junction. These findings are consistent with the established principle that optimum Cd-free buffers remain sufficiently thin to minimize parasitic optical absorption while maintaining continuous heterojunction coverage [9]. An optimum buffer thickness of 0.05 μm is therefore selected. The same nominal thickness was selected for the MgZnO layer in an optimized MgZnO/i-CIGS/CIGS structure, where it was combined with a 4 μm absorber and yielded the best performance at 290 K [21]. This agreement is qualitative rather than universal because the absorber, band offsets, contacts, and simulation tool differ. A comparable optical-thickness penalty was observed in simulated CdTe cells, for which thinning Cd-free ZnO, ZnSe, and ZnS buffers to approximately 0.01 μm improved performance and the optimized ZnS- and ZnSe-buffered devices achieved efficiencies of 25.23% and 25.04%, respectively [7]. Collectively, these studies show that an unnecessarily thick buffer reduces useful photon flux and can increase transport and recombination losses.

3.3.2 ZnO Window Layer Thickness

The ZnO window thickness w_{ZnO} is swept from 0.02 to 0.2 μm with the 4 μm absorber and 0.05 μm buffer fixed. Figure 6 summarizes the resulting trends.

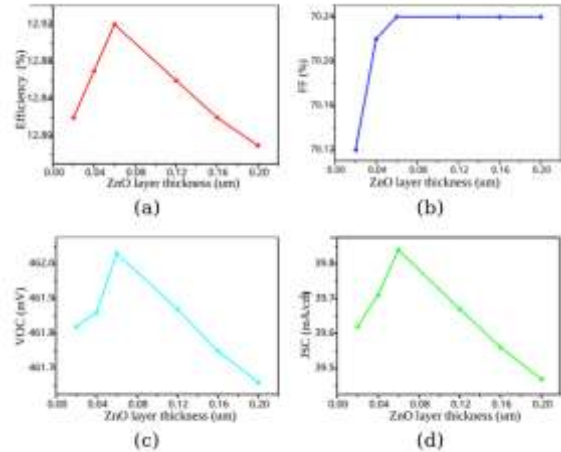


Figure 6. Device performance parameters as a function of ZnO window layer thickness: (a) η , (b) FF, (c) V_{oc} , (d) J_{sc} .

A clear maximum in $\eta \approx 12.92\%$ and $J_{sc} \approx 39.8 \text{ mA cm}^{-2}$ emerges around $w_{ZnO} = 0.06$ to 0.08 μm ; both quantities decrease at greater thickness because optical absorption and resistive losses accumulate in the ZnO window. V_{oc} peaks at $\approx 462 \text{ mV}$ near

0.08 μm before declining, whereas FF stabilizes above $\approx 70.24\%$ for w_{ZnO} above 0.04 μm , confirming that a minimum ZnO thickness is required to provide adequate lateral conductivity. Experimental ZnO films have exhibited high visible transparency, with an average transmittance of approximately 85% and band gaps in the 3.24 to 3.37 eV range under Al/Mg doping [39]. Configuration-dependent ZnO/TiO₂ thin films likewise maintained more than 60% transparency over 350 to 900 nm, while their band gaps varied with single-layer, composite, and bilayer architecture [40]. Although those material studies do not reproduce the present TCO stack, they reinforce that film composition, thickness, and interfaces jointly determine optical transmission. A related CZTSSe investigation showed that the thickness of Al-doped ZnO transparent electrodes can modify thin-film interference and optical response [41]. Hybrid CIGS/ASnI₂Br simulations similarly identified parasitic ultraviolet absorption and nonideal resistances as window-stack loss channels [24], while bifacial perovskite modeling compared ZnOS and MZO electron-transport layers through their effects on energy alignment, recombination, and stability [26]. A ZnO window thickness of 0.06 μm is selected for the final optimized structure. Thus, the window-layer optimum reflects a device-level compromise between transparency and sheet-conduction requirements rather than either property in isolation.

3.4 Optimization of CZTSe Acceptor Doping Density

The p-type doping N_A in the CZTSe absorber is varied from 1×10^{15} to $5 \times 10^{15} \text{ cm}^{-3}$. Figure 7 summarizes the resulting trends.

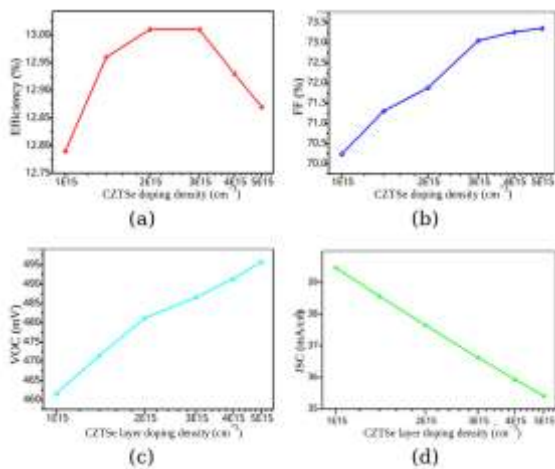


Figure 7. Device performance parameters as a function of CZTSe acceptor doping density N_A : (a) η , (b) FF, (c) V_{oc} , (d) J_{sc} .

V_{oc} increases monotonically from $\approx 460 \text{ mV}$ to $\approx 495 \text{ mV}$ across this range, driven by the deepening junction built-in potential at higher acceptor concentration. FF likewise increases from $\approx 70\%$ to $\approx 73.2\%$, consistent with a stronger depletion-region field and more efficient charge extraction over the investigated interval. A comparable qualitative dependence of field-assisted extraction on doping has been reported in a different InGaP/GaAs dual-junction architecture [42], although the material and junction physics differ. However, J_{sc} exhibits a non-monotonic response, peaking near $\approx 39.5 \text{ mA cm}^{-2}$ at $N_A \approx 2 \times 10^{15} \text{ cm}^{-3}$ and subsequently declining at higher doping because the depletion width and minority-carrier diffusion length are reduced by ionized-impurity scattering and SRH recombination at dopant-related trap states. The resulting η peaks near $\approx 13.2\%$ at $N_A \approx 3 \times 10^{15} \text{ cm}^{-3}$ before diminishing. In the final optimized device, $N_A = 1.4 \times 10^{15} \text{ cm}^{-3}$ is selected within the lower-doping interval to preserve the higher J_{sc} contribution while maintaining substantially improved V_{oc} and FF relative to the baseline, in accordance with the observed J_{sc} - V_{oc} trade-off. The strong influence of acceptor density on V_{oc} agrees qualitatively with the CdS/CZTSSe analysis in [9], although that study reported an optimum CZTSSe doping density of 10^{17} cm^{-3} . Comparable architecture-specific trends appear in other uploaded simulations: $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ optimization balanced voltage improvement against photocurrent retention [23]; a hybrid CIGS/ASnI₂Br cell was optimized over an acceptor range of 10^{12} - 10^{15} cm^{-3} [24]; and lead-free CsSnI_3 studies improved performance through doping optimization, reaching 20.25% at 10^{17} cm^{-3} in one architecture [25] and 23.14% after doping optimization in another [27]. These values should not be ranked directly against the present CZTSe result because the absorber chemistry, defect densities, interfaces, carrier lifetimes, and transport layers differ. The comparisons nevertheless confirm that doping affects built-in potential, depletion width, recombination, and collection simultaneously, so its optimum must be determined within the complete device structure.

3.5 Comparison of Baseline and Fully Optimized J-V Characteristics

The cumulative effect of all structural and doping optimizations is summarized in Table 4 and Figure 8, comparing the baseline CZTSe/Zn(O_{0.4}S_{0.6})/ZnO cell ($w_{\text{CZTSe}} = 2 \mu\text{m}$, $w_{\text{buf}} = 0.05 \mu\text{m}$, $w_{\text{ZnO}} = 0.2 \mu\text{m}$, $N_A = 10^{15} \text{ cm}^{-3}$) with the fully optimized configuration ($w_{\text{CZTSe}} = 4 \mu\text{m}$, $w_{\text{buf}} = 0.05 \mu\text{m}$, w_{ZnO}

$= 0.06 \mu\text{m}$, $N_A = 1.4 \times 10^{15} \text{ cm}^{-3}$, $N_D (\text{ZnO}) = 10^{19} \text{ cm}^{-3}$.

Table 4. Comparison of performance metrics for the baseline and fully optimized CZTSe/Zn(O_{0.4}S_{0.6})/ZnO cell.

Metric	Baseline Cell	Optimized Cell	Absolute Gain
J_{sc} (mA cm ⁻²)	39.47	41.20	+1.73
V_{oc} (mV)	461.66	483.08	+21.42
FF (%)	70.24	71.02	+0.78
η (%)	12.79	14.13	+1.34

The 1.34 percentage-point absolute efficiency gain is attributable to three physically distinct mechanisms: (i) the 4 μm absorber increases the effective optical absorption volume without exceeding the collection-length constraint, driving the J_{sc} improvement of +1.73 mA cm⁻². The role of absorber thickness in photocurrent generation has also been modeled for a different graded CdZnTe system [43], although the present numerical gain is specific to CZTSe; (ii) the refined Zn(O_{0.4}S_{0.6})/CZTSe CBO, maintained in a near-neutral to slightly spike-like configuration, suppresses interface recombination and contributes to the V_{oc} gain. A related SnS/Zn(O,S) study likewise demonstrates the sensitivity of carrier transport to heterojunction band alignment [44], but its band offsets cannot be transferred quantitatively to CZTSe; and (iii) the optimized acceptor doping strengthens the built-in electric field and reduces SRH-limited bulk losses, yielding improved V_{oc} and FF. Similar doping-recombination trade-offs have been numerically analyzed in different Sb₂S₃/Sb₂Se₃ absorber systems [45], with architecture-specific optimum values. In the CdS-buffered CZTSSe study of [9], combined thickness and doping optimization produced a larger absolute PCE increase, from 12.73% to 18.75%. A direct ranking is not meaningful because the buffer material, baseline structure, defect parameters, and optimization ranges differ; nevertheless, both studies identify photon absorption, junction electrostatics, and recombination as coupled design variables. The same need to balance absorber thickness and doping has also been observed in

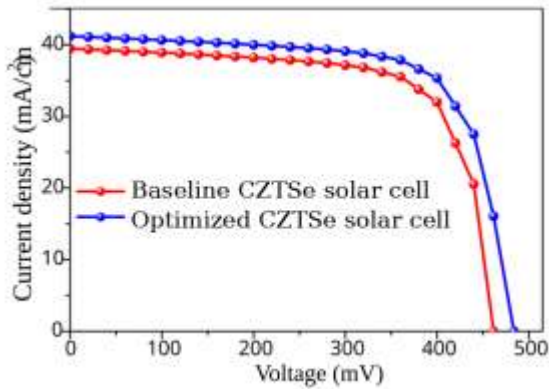


Figure 8. J-V characteristics of the baseline and fully optimized CZTSe/Zn(O_{0.4}S_{0.6})/ZnO solar cells. Annotations indicate J_{sc} , V_{oc} , and maximum power point for each curve.

simulated CZTSSe-containing tandem cells [36], although current matching introduces an additional constraint that is absent from the present single-junction device. More broadly, the bifacial perovskite study in [26] showed that material selection, bandgap, defect density, thickness, and parasitic resistances must be co-optimized; this supports the present cumulative strategy while remaining quantitatively distinct from CZTSe.

3.6 Temperature Dependence of the Optimized Cell

Temperature-dependent simulations of the optimized cell were performed from 240 to 350 K to assess thermal robustness under realistic operating conditions. As temperature increases, V_{oc} declines approximately linearly from ≈ 610 mV at 240 K to ≈ 375 mV at 350 K; FF drops from $\approx 74\%$ to $\approx 65\%$; and η decreases sharply, consistent with the temperature dependence of the diode saturation current. These trends are summarized in Figure 9.

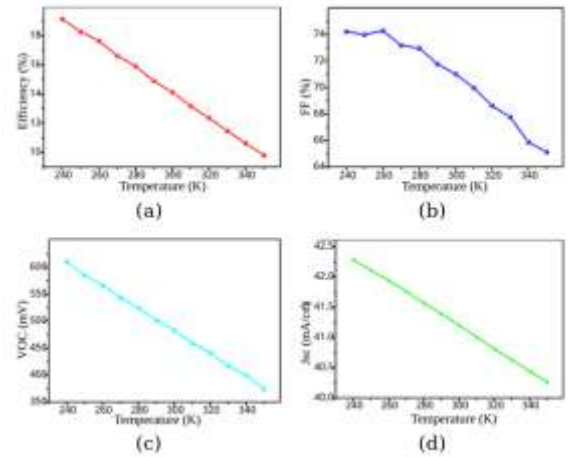


Figure 9. Temperature-dependent performance parameters of the optimized CZTSe/Zn(O_{0.4}S_{0.6})/ZnO cell (240 to 350 K): (a) η , (b) FF, (c) V_{oc} , (d) J_{sc} .

The governing relation is:

$$V_{oc} \approx \frac{kT}{q} \ln \left(\frac{I_{ph}}{I_0} + 1 \right) \quad (7)$$

where I_{ph} is the photocurrent and I_0 is the reverse saturation current [46]. Increasing temperature raises the intrinsic carrier concentration n_i and therefore I_0 , directly suppressing V_{oc} . Simultaneously, enhanced phonon scattering and increased trap activation intensify SRH and Auger recombination, degrading both FF and η [47]. The mild reduction in J_{sc} from ≈ 42 to ≈ 40 mA cm⁻²

across 240 to 350 K is attributable to increased carrier recombination rather than to spectral changes, confirming that SRH-dominated bulk recombination is the dominant thermally activated loss mechanism in the optimized CZTSe absorber. Thermal management and low-temperature operation (260 to 280 K) would provide an absolute efficiency gain of approximately 2 to 3 percentage points. The direction of this trend is consistent with independent simulations of CdTe [46], CdS/CZTSSe [9], CGS/CIGS [1], and CGS/CZTSSe [36] cells, as well as the CZTS/CIGS tandem analysis in [47]. The newly considered MgZnO/CIGS study reported its highest simulated efficiency of 25.63% at 290 K [21], whereas the hybrid CIGS/ASnI₂Br study explicitly evaluated 260 to 340 K and reported comparatively stable operation across that interval [24]. These results reinforce the need to evaluate temperature within each complete layer stack; the exact coefficient and optimum cannot be transferred because every study adopts different band gaps, defect models, contacts, and temperature-dependent material parameters.

4. Conclusions

This work numerically optimized a fully Cd-free glass/Mo/p-CZTSe/n-Zn(O_xSi_{1-x})/n-ZnO/ITO solar cell using Silvaco ATLAS. The buffer composition was the principal factor controlling the CZTSe/Zn(O,S) conduction-band alignment. At $x = 0.4$, Zn(O_{0.4}Si_{0.6}) ($E_g = 2.72$ eV and $\chi = 4.08$ eV) produced a near-neutral to slightly positive offset that limited interface recombination without creating a significant electron-extraction barrier. Lower oxygen fractions formed an excessive spike, whereas higher fractions produced a cliff-like alignment and reduced the fill factor.

The optimized structure used $w_{\text{CZTSe}} = 4$ μm , $w_{\text{buf}} = 0.05$ μm , $w_{\text{ZnO}} = 0.06$ μm , and $N_A = 1.4 \times 10^{15}$ cm^{-3} . It achieved $\eta = 14.13\%$, $J_{sc} = 41.20$ mA cm^{-2} , $V_{oc} = 483.08$ mV, and $\text{FF} = 71.02\%$, compared with 12.79% for the baseline cell. The gain resulted from increased light harvesting, reduced front-layer losses, and improved carrier collection. Increasing temperature from 240 to 350 K progressively reduced V_{oc} , FF, and efficiency because of the higher saturation current and stronger trap-assisted recombination.

These numerical predictions assume literature-derived parameters, uniform defect distributions, ideal ohmic contacts, and one-dimensional transport. Experimental validation should focus on controlled Zn(O,S) deposition, direct band-offset and interface-defect measurements, and calibrated multidimensional modeling of grain boundaries,

compositional nonuniformity, thermal cycling, and operational stability.

Author Statements:

- **Ethical approval:** The conducted research is not related to either human or animal use.
- **Conflict of interest:** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
- **Acknowledgement:** The authors declare that they have nobody or no company to acknowledge.
- **Author contributions:** The authors declare that they have equal rights in this paper.
- **Funding information:** The authors declare that there is no funding to be acknowledged.
- **Data availability statement:** The data supporting the findings of this study are available from the corresponding author upon reasonable request.

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