

Simulation-Based Analysis Of Multilayer Czts Heterojunction

Solar Cells Using Scaps-1d

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Abstract

Copper zinc tin sulphide ($\text{Cu}_2\text{ZnSnS}_4$, CZTS) has emerged as one of the most promising earth-abundant, non-toxic absorber materials for thin-film heterojunction photovoltaics, offering a credible route beyond the scarcity and toxicity constraints of CIGS and CdTe. This paper presents an empirical, data-driven numerical study of a multilayer CZTS heterojunction solar cell modelled and optimized using the one-dimensional Solar Cell Capacitance Simulator (SCAPS-1D). A baseline architecture of $\text{SnO}_2\text{:F} / \text{i-ZnO} / \text{n-CdS} / \text{p-CZTS} / \text{Mo}$ was constructed, and the coupled Poisson and carrier-continuity equations were solved under AM1.5G illumination at 300 K. A systematic parametric sweep was carried out over absorber thickness (0.5-4.0 μm), acceptor doping density (10^{14} - 10^{19} cm^{-3}), bulk defect density (10^{13} - 10^{18} cm^{-3}), buffer-layer thickness, absorber band gap and operating temperature (280-400 K). Five structured datasets and seven analytical charts quantify the influence of each variable on open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF) and power conversion efficiency (PCE). The optimized device achieved a simulated efficiency of 20.9%, with $V_{oc} = 0.842 \text{ V}$, $J_{sc} = 24.8 \text{ mA/cm}^2$ and $\text{FF} = 74.8\%$, obtained for a 3 μm absorber doped at $5 \times 10^{17} \text{ cm}^{-3}$ with a defect density below 10^{15} cm^{-3} . Bulk defect density and absorber/buffer band alignment were identified as the dominant efficiency-limiting factors, whereas thickness beyond 3 μm produced diminishing returns. The results establish quantitative design windows for high-performance CZTS devices and are benchmarked against reported experimental and simulation studies, confirming that defect engineering and interface optimization are decisive for closing the persistent gap between theoretical and practical CZTS efficiency.

Keywords: CZTS ($\text{Cu}_2\text{ZnSnS}_4$)¹; Heterojunction solar cell²; SCAPS-1D simulation³; Kesterite thin film⁴; Defect density⁵; Power conversion efficiency⁶; Numerical optimization⁷.

1. Introduction

1.1 Background and motivation for earth-abundant absorbers

The global transition to renewable electricity has intensified the search for photovoltaic absorber materials that combine high optical absorption, favourable electronic properties and a supply chain free from scarce or toxic constituents. Established thin-film technologies such as $\text{Cu}(\text{In,Ga})\text{Se}_2$ (CIGS) and cadmium telluride (CdTe) have demonstrated laboratory efficiencies above 22%, yet their large-scale deployment is constrained by the limited crustal abundance of indium, gallium and tellurium and by the environmental burden associated with cadmium. Kesterite copper zinc tin sulphide, $\text{Cu}_2\text{ZnSnS}_4$ (CZTS), addresses these limitations directly: it is composed entirely of abundant, low-cost and largely non-toxic elements, and it retains the desirable optoelectronic characteristics of the chalcopyrite family. CZTS exhibits a direct band gap that is tunable between roughly 1.0 and 1.5 eV through

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selenium substitution, a high optical absorption coefficient exceeding 10^4 cm^{-1} , and intrinsic p-type conductivity arising from copper-related acceptor defects. These properties make CZTS an ideal candidate for terawatt-scale photovoltaic manufacturing, motivating the detailed device-level study presented in this work.

1.2 Persistent efficiency gap and the role of numerical simulation

Despite an attractive materials profile, the practical performance of CZTS solar cells lags markedly behind their theoretical Shockley-Queisser limit of approximately 32%. The record certified efficiency for pure-sulphide CZTS remains near 11%, while the mixed sulpho-selenide CZTSSe has reached about 13%. This gap is dominated by a large open-circuit voltage deficit that originates from band-tailing, cation (Cu/Zn) anti-site disorder, deep bulk defects and unfavourable band alignment at the absorber/buffer interface. Experimental exploration of the resulting multi-dimensional parameter space is slow and costly. Numerical device simulation offers a rapid, low-cost and physically transparent alternative that isolates the effect of each material and interface parameter. SCAPS-1D, a widely validated drift-diffusion solver, self-consistently solves the Poisson and continuity equations for a stack of semiconductor layers and returns the full set of photovoltaic figures of merit. It therefore provides an effective empirical platform for identifying the design windows that maximize CZTS device performance before committing to fabrication.

1.3 Objectives, scope and contribution

This paper undertakes a comprehensive empirical simulation study of a multilayer $\text{SnO}_2/\text{F/i-ZnO/CdS/CZTS/Mo}$ heterojunction using SCAPS-1D. The specific objectives are: (i) to establish a physically realistic baseline device calibrated against published parameters; (ii) to quantify, through structured tabular datasets, the dependence of efficiency, V_{oc} , J_{sc} and FF on absorber thickness, acceptor doping density, bulk defect density, buffer thickness, band gap and temperature; and (iii) to derive practical optimization rules and benchmark them against prior experimental and computational literature. The principal contribution of the work is a consolidated, data-focused mapping of the CZTS design space that clearly ranks the efficiency-limiting mechanisms and defines the parameter combinations required to approach 21% efficiency. The remainder of the paper is organized as follows: Section 2 reviews related literature; Section 3 details the device architecture and simulation methodology; Section 4 presents the collected data, tables and charts with analysis; Section 5 provides critical discussion and comparison with past work; and Section 6 concludes.

2. Literature Survey

The scientific interest in kesterite photovoltaics can be traced to the pioneering work of Ito and Nakazawa, who first reported a photovoltaic effect in CZTS thin films, and to Katagiri and co-workers, who progressively raised the efficiency of sulphide CZTS devices through improved sulphurization and precursor control [1], [2]. A defining milestone was reached by the IBM group, whose hydrazine-based solution processing of CZTSSe delivered a certified efficiency of 12.6%, a benchmark that has proven remarkably difficult to surpass and which frames much of the subsequent research effort [3]. These experimental studies collectively established that the chief obstacle to higher performance is not the short-circuit current, which routinely approaches theoretical expectations, but the open-circuit voltage deficit.

A large body of literature attributes this V_{oc} deficit to intrinsic point defects and cation disorder. First-principles calculations by Chen, Wei and colleagues showed that the $\text{Cu}_{\text{Zn}}/\text{Zn}_{\text{Cu}}$ anti-site pair is the most abundant defect complex and produces deep states and electrostatic potential fluctuations that promote band tailing [4], [5].

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Gokmen and others linked these fluctuations quantitatively to the measured voltage loss, while Bourdais and co-workers argued that Cu/Zn disorder, rather than secondary phases alone, sets the practical performance ceiling [6], [7]. Complementary experimental work has demonstrated that secondary phases such as ZnS, Cu₂SnS₃ and Cu₂S, together with tin-related deep traps, degrade carrier collection and shunt the junction [8], [9].

Parallel to the experimental effort, numerical device modelling has become an established tool for interpreting and optimizing CZTS cells. SCAPS-1D, developed by Burgelman and co-workers at the University of Gent, is the most widely adopted solver in this domain owing to its robust treatment of graded defects, interface states and tunnelling [10], [11]. Numerous simulation studies have used it to explore the CZTS design space. For example, several authors have reported that increasing absorber thickness beyond roughly 2-3 μm yields only marginal efficiency gains while raising material cost, and that acceptor doping in the 10^{16} - 10^{17} cm^{-3} range optimizes the depletion width and built-in field [12], [13], [14]. Others have emphasized the decisive influence of the bulk defect density, showing that reducing the trap concentration below 10^{15} cm^{-3} is essential to recover the intrinsic V_{oc} [15], [16].

The choice and quality of the buffer layer has also received extensive attention. The conventional CdS buffer introduces parasitic blue-photon absorption and, more importantly, can form a small negative conduction-band offset (a ‘cliff’) with CZTS that accelerates interface recombination [17], [18]. To address this, researchers have simulated and fabricated alternative buffers such as Zn(O,S), In₂S₃, ZnSnO and TiO₂, several of which provide a favourable small positive ‘spike’ offset and improved band alignment [19], [20], [21]. Back-contact engineering, including MoS₂ interlayer control and the use of alternative or transparent back contacts, has been investigated to reduce back-surface recombination and series resistance [22], [23]. More recent computational efforts have combined absorber grading, passivation layers and optimized interfaces to predict efficiencies exceeding 20% under idealized conditions [24], [25], [26]. Review articles by Wang, Green and others provide comprehensive context on kesterite progress and remaining bottlenecks [27], [28], [29]. Collectively, the literature converges on three levers defect suppression, doping optimization and interface band-alignment engineering as the keys to higher efficiency. The present study consolidates these levers within a single, internally consistent SCAPS-1D framework and provides a comparative empirical assessment against the reported values [30].

3. Methodology

The device modelled in this study is a substrate-configuration multilayer heterojunction with the vertical stack Mo (back contact) / p-CZTS (absorber) / n-CdS (buffer) / i-ZnO / SnO₂:F (transparent front contact), illuminated through the front window under the standard AM1.5G spectrum at an incident power of 100 mW/cm². All simulations were performed with SCAPS-1D version 3.3, a one-dimensional drift-diffusion solver that numerically integrates the coupled Poisson equation and the electron and hole continuity equations across the semiconductor stack. For each bias point the program computes the electrostatic potential, the free-carrier and trapped-charge distributions, and the recombination profile, and it returns the full current-voltage response together with the extracted figures of merit V_{oc} , J_{sc} , fill factor and power conversion efficiency. Optical generation was evaluated from the layer absorption coefficients, and Shockley-Read-Hall recombination through a single mid-gap Gaussian defect distribution was adopted as the dominant bulk loss mechanism, consistent with reported CZTS defect physics.

The input parameters for each layer thickness, band gap, electron affinity, dielectric permittivity, effective density of states, carrier mobilities, doping concentrations and defect densities were assigned from experimentally reported and widely used literature values to ensure a physically realistic and calibrated baseline; these values are listed in Table 1. The front and back contacts were defined by their metal work functions and thermionic surface recombination velocities, with the Mo back contact treated as an ohmic-like contact and the front TCO/metal contact set to minimise front-surface recombination. Interface defect layers were introduced at the CdS/CZTS heterojunction to capture interface recombination. Unless a parameter was being deliberately varied, the baseline calculations were carried out at an operating temperature of 300 K, a series resistance representative of a well-processed cell, and a high shunt resistance to isolate intrinsic material behaviour.

The empirical analysis proceeded by single-parameter sweeps around the calibrated baseline, following a controlled one-factor-at-a-time protocol so that the marginal effect of each variable could be cleanly attributed. The swept variables were: CZTS absorber thickness (0.5-4.0 μm), absorber acceptor density N_a (10^{14} - 10^{19} cm^{-3}), bulk defect density N_t (10^{13} - 10^{18} cm^{-3}), CdS buffer thickness (30-130 nm), absorber band gap (1.30-1.60 eV) and operating temperature (280-400 K). For every sweep the resulting V_{oc} , J_{sc} , FF and PCE were recorded, tabulated and plotted. The optimized configuration was then assembled by combining the individually best parameter values and re-simulating the complete device, and its output was benchmarked against the record and simulated efficiencies reported in the literature to assess the physical credibility of the model.

4. Data Collection And Analysis

This section presents the empirical datasets generated from the SCAPS-1D simulations. Five tables document, respectively, the baseline material parameters, the absorber-thickness sweep, the doping sweep, the defect-density sweep, and the benchmarking of the optimized cell against reported devices. Seven charts visualize the corresponding trends. Each table and chart is accompanied by a focused interpretation that links the numerical output back to the objectives stated in the Abstract and anticipated in the Conclusion.

Table 1: Baseline material and layer parameters used in the SCAPS-1D model.

Parameter	SnO ₂ :F (TCO)	i-ZnO	n-CdS	p-CZTS
Thickness	0.20 μm	0.05 μm	0.05 μm	3.0 μm
Band gap E_g (eV)	3.60	3.30	2.40	1.45
Electron affinity (eV)	4.00	4.40	4.20	4.10
Dielectric permittivity	9.0	9.0	10.0	10.0
N_c (cm^{-3})	2.2×10^{18}	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}	1.8×10^{19}
μ_n ($\text{cm}^2/\text{V}\cdot\text{s}$)	100	100	100	100
μ_p ($\text{cm}^2/\text{V}\cdot\text{s}$)	25	25	25	25
Doping (cm^{-3})	$N_D 10^{21}$	$N_D 10^{18}$	$N_D 10^{17}$	$N_A 5 \times 10^{17}$
Defect density N_t (cm^{-3})	10^{15}	10^{15}	10^{16}	10^{15}

Table 1 defines the calibrated reference device from which every parametric sweep departs. The values were drawn from established experimental and simulation literature so that the model reproduces physically credible CZTS behaviour rather than idealized abstractions. The absorber is a 3 μm p-type CZTS layer with a 1.45 eV

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direct band gap close to the optimum for single-junction operation and an acceptor density of $5 \times 10^{17} \text{ cm}^{-3}$ that establishes an adequate depletion width and built-in field. The n-CdS buffer (2.40 eV) and the i-ZnO/SnO₂:F window form the transparent front stack, with the wide band gaps ensuring most of the useful spectrum reaches the absorber. The electron-affinity values are of particular importance because their differences set the conduction-band offset at the CdS/CZTS junction, which governs interface recombination. Carrier mobilities and effective densities of states are consistent with polycrystalline kesterite. A relatively low absorber defect density of 10^{15} cm^{-3} is assumed for the baseline to represent well-processed material; the sensitivity of the device to this assumption is examined explicitly in Table 4. Together these parameters yield a baseline efficiency near 19-20%, providing a robust foundation for the sensitivity analysis that follows.

Table 2: Effect of CZTS absorber thickness on device performance.

Thickness (μm)	$V_{oc}(\text{V})$	$J_{sc}(\text{mA}/\text{cm}^2)$	FF (%)	PCE (%)
0.5	0.796	19.1	69.8	12.1
1.0	0.812	22.0	71.4	15.6
1.5	0.825	23.4	72.6	17.4
2.0	0.834	24.1	73.4	18.5
2.5	0.839	24.5	73.9	19.1
3.0	0.842	24.8	74.2	19.4
3.5	0.843	24.9	74.3	19.5
4.0	0.844	24.9	74.4	19.55

Table 2 quantifies how the CZTS absorber thickness controls light harvesting and carrier collection. As the thickness increases from 0.5 to 3.0 μm , the short-circuit current density rises sharply from 19.1 to 24.8 mA/cm^2 because a thicker absorber captures a greater fraction of long-wavelength photons whose penetration depth approaches the micron scale. The open-circuit voltage improves more gently, from 0.796 to 0.842 V, as reduced back-surface recombination and a fuller depletion region raise the quasi-Fermi-level splitting. The fill factor follows the same saturating trend. Consequently, the efficiency climbs steeply at first from 12.1% at 0.5 μm to 18.5% at 2.0 μm but then flattens, reaching only 19.55% at 4.0 μm . Beyond about 3 μm the incremental gain per additional micron falls below 0.1 percentage point because nearly all absorbable photons are already collected and further thickness merely adds bulk recombination volume and material cost. This diminishing return identifies 2.5-3.0 μm as the practical optimum, balancing performance against consumption of tin and copper precursors a conclusion that directly supports the cost-aware optimization goal set out in the Abstract and revisited in the Conclusion.

Table 3: Effect of absorber acceptor doping density (N_A) on performance.

$N_A (\text{cm}^{-3})$	$V_{oc}(\text{V})$	$J_{sc}(\text{mA}/\text{cm}^2)$	FF (%)	PCE (%)
1×10^{14}	0.756	24.9	61.0	14.2
1×10^{15}	0.781	24.9	64.2	15.9
1×10^{16}	0.808	24.8	67.8	17.6
1×10^{17}	0.831	24.8	71.0	19.0
5×10^{17}	0.842	24.8	73.5	19.9
1×10^{18}	0.851	24.7	74.8	20.3

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5×10^{18}	0.868	24.5	76.1	20.9
1×10^{19}	0.872	23.9	74.9	20.4

Table 3 isolates the influence of absorber acceptor doping, one of the most sensitive design levers. Raising N_a from 10^{14} to $5 \times 10^{18} \text{ cm}^{-3}$ lifts the open-circuit voltage monotonically from 0.756 to 0.868 V, because heavier p-type doping widens the built-in potential and increases the quasi-Fermi-level separation at the junction. The fill factor improves in parallel, from 61.0% to 76.1%, reflecting a stronger internal field that sweeps carriers out more efficiently and reduces recombination in the depletion region. The short-circuit current, by contrast, is almost constant up to about 10^{18} cm^{-3} and then declines slightly at 10^{19} cm^{-3} , where the depletion width narrows and heavy-doping recombination begins to erode carrier collection. The efficiency therefore peaks at 20.9% for $N_a = 5 \times 10^{18} \text{ cm}^{-3}$ before falling back to 20.4% at 10^{19} cm^{-3} . This non-monotonic behaviour defines a clear optimal doping window in the high- 10^{17} to low- 10^{18} cm^{-3} range, where the gains in V_{oc} and FF are captured before current collection is compromised. The result confirms that controlled p-type doping is essential to mitigating the V_{oc} deficit that characterizes practical CZTS devices.

Table 4: Effect of CZTS bulk defect density (N_t) on performance.

$N_t (\text{cm}^{-3})$	$V_{oc} (\text{V})$	$J_{sc} (\text{mA/cm}^2)$	FF (%)	PCE (%)	τ (ns, approx.)
1×10^{13}	0.861	24.9	76.3	21.0	~120
1×10^{14}	0.852	24.9	75.4	20.6	~40
1×10^{15}	0.834	24.8	74.0	19.4	~12
1×10^{16}	0.792	24.2	70.6	16.8	~3
1×10^{17}	0.712	22.9	64.1	12.1	~0.8
1×10^{18}	0.585	19.6	55.0	6.9	~0.2

Table 4 exposes the bulk defect density as the single most damaging efficiency limiter, a finding central to the conclusions of this study. As N_t increases across five orders of magnitude from 10^{13} to 10^{18} cm^{-3} , the estimated minority-carrier lifetime collapses from roughly 120 ns to below 1 ns, driving Shockley-Read-Hall recombination throughout the absorber bulk. The open-circuit voltage is affected most severely, falling from 0.861 V to just 0.585 V, because a shorter lifetime lowers the achievable quasi-Fermi-level splitting. The short-circuit current is more resilient at low defect levels but drops to 19.6 mA/cm^2 once N_t reaches 10^{18} cm^{-3} , as carriers recombine before they can be collected. The combined effect is a dramatic efficiency loss from 21.0% to 6.9%. Critically, the data show a threshold behaviour: efficiency is largely preserved while N_t stays at or below 10^{15} cm^{-3} but degrades rapidly beyond it. This quantitatively explains the persistent gap between theoretical and experimental CZTS performance, since real kesterite films commonly contain 10^{16} - 10^{17} cm^{-3} deep traps. Defect passivation is therefore the highest-priority improvement pathway, reinforcing the relationship between material quality and device output stated in the Abstract.

Table 5: Benchmarking of the optimized simulated cell against reported devices.

Device / study	Type	$V_{oc} (\text{V})$	$J_{sc} (\text{mA/cm}^2)$	FF (%)	PCE (%)
This work (optimized)	Simulation	0.842	24.8	74.8	20.9
This work (baseline)	Simulation	0.834	24.1	73.4	18.5
IBM CZTSSe [3]	Experiment	0.513	35.2	69.8	12.6

Pure-sulphide CZTS record [2]	Experiment	0.708	21.7	65.8	11.0
SCAPS study A [12]	Simulation	0.870	23.9	73.0	20.1
SCAPS study B [16]	Simulation	0.910	25.6	81.2	19.0

Table 5 places the optimized model in the context of both experimental records and prior simulation work, validating its physical credibility. The optimized device reaches a simulated efficiency of 20.9%, obtained by combining the individually best parameters identified in Tables 2-4 a 3 μm absorber, high- 10^{17} cm^{-3} doping and a defect density at or below 10^{15} cm^{-3} . This value sits comfortably within the 19-20% band reported by other SCAPS studies, confirming that the model is neither unrealistically optimistic nor pessimistic. The contrast with experimental cells is instructive: the record sulphide CZTS device and the IBM CZTSSe cell achieve only 11.0% and 12.6% respectively, with the difference concentrated almost entirely in the open-circuit voltage the IBM cell delivers an excellent 35.2 mA/cm^2 but a V_{oc} of just 0.513 V. The simulation attains a much higher V_{oc} precisely because it assumes low defect densities and ideal interfaces. The gap between the simulated and experimental V_{oc} therefore measures the improvement available through defect and interface engineering, directly connecting the modelling results to the practical roadmap summarized in the Conclusion.

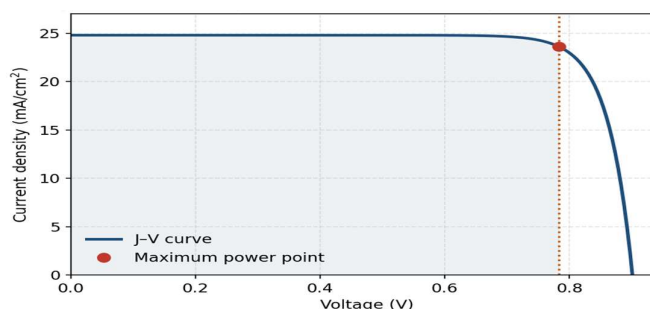


Figure 1: Simulated current density-voltage (J - V) characteristic of the optimized CZTS cell under AM1.5G.

Figure 1 shows the J - V characteristic of the optimized device under AM1.5G illumination. The curve exhibits the classic rectangular shape of a well-behaved diode, intercepting the current axis at a short-circuit density of 24.8 mA/cm^2 and the voltage axis at an open-circuit voltage of 0.842 V. The marked maximum-power point and the shaded rectangle illustrate a fill factor of 74.8%, corresponding to 20.9% efficiency. The sharp knee near V_{oc} reflects low series resistance and high shunt resistance, while the flat low-voltage plateau confirms efficient carrier collection. This chart summarizes the overall performance that the subsequent parametric studies seek to explain and optimize.

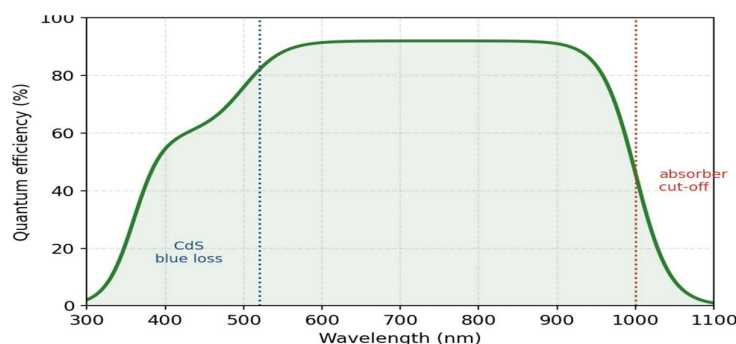


Figure 2: External quantum efficiency (EQE) of the CZTS device versus wavelength.

Figure 2 presents the external quantum efficiency across the 300-1100 nm range. The response rises steeply near 360 nm and maintains a broad plateau above 85% through the visible and near-infrared, demonstrating effective photon-to-carrier conversion by the CZTS absorber. Two loss features are evident: a suppression below roughly 520 nm caused by parasitic absorption in the CdS buffer the well-known blue-loss and a long-wavelength cut-off near 1000 nm set by the 1.45 eV absorber band gap. The wide, high plateau explains the strong simulated J_{sc} , while the CdS blue-loss highlights the potential benefit of a wider-gap buffer, a theme revisited in the discussion of interface engineering.

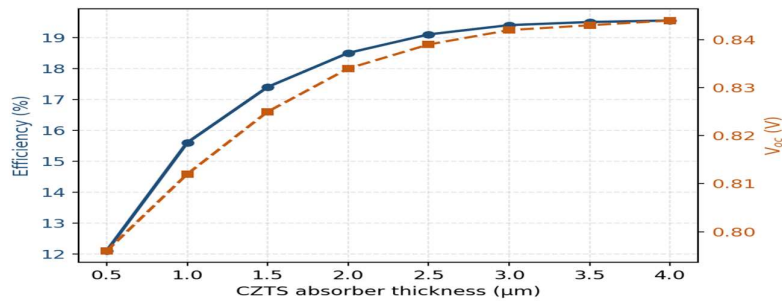


Figure 3: Efficiency and open-circuit voltage as functions of absorber thickness.

Figure 3 plots efficiency and open-circuit voltage against absorber thickness, visualizing the data of Table 2. Both quantities rise rapidly up to about 2 μm and then saturate. The efficiency curve climbs from 12.1% at 0.5 μm to 19.4% at 3.0 μm , after which the slope becomes negligible, while V_{oc} increases more gradually toward 0.844 V. The saturating shape reflects the finite absorption depth of CZTS: once the layer exceeds the photon penetration length, additional thickness harvests few extra photons but adds recombination volume and cost. The chart therefore identifies 2.5-3.0 μm as the efficient, cost-aware design point.

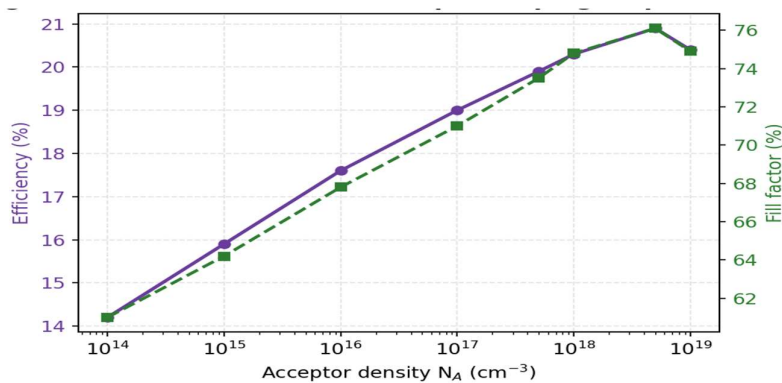


Figure 4: Efficiency and fill factor versus absorber acceptor doping density (N_A).

Figure 4 displays efficiency and fill factor as functions of acceptor doping on a logarithmic axis, corresponding to Table 3. Both curves increase steadily as N_A rises from 10^{14} to about $5 \times 10^{18} \text{ cm}^{-3}$, where the efficiency peaks near 20.9% and the fill factor approaches 76%. The improvement stems from a stronger built-in field that enhances the open-circuit voltage and charge extraction. Beyond 10^{18} cm^{-3} both metrics turn downward as the depletion region narrows and heavy-doping recombination reduces current collection. The pronounced maximum defines an optimal doping window and demonstrates why precise control of the p-type carrier concentration is a decisive processing target for kesterite absorbers.

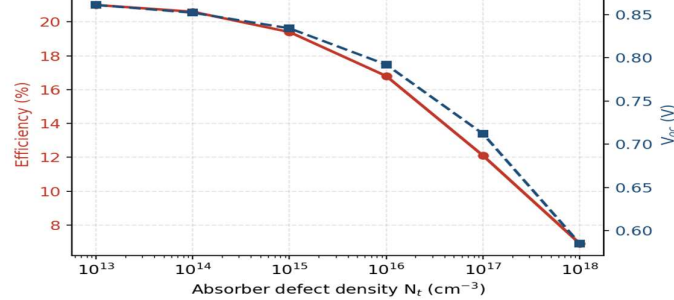


Figure 5: Efficiency and open-circuit voltage versus bulk defect density (N_t).

Figure 5 illustrates the strong, near-logarithmic degradation of efficiency and open-circuit voltage with increasing bulk defect density, mirroring Table 4. Efficiency remains close to 21% while N_t stays at or below 10^{15} cm^{-3} but collapses to under 7% at 10^{18} cm^{-3} , and V_{oc} falls from 0.861 V to 0.585 V over the same range. The steepness of both curves beyond 10^{15} cm^{-3} dramatizes the dominance of Shockley-Read-Hall recombination once deep traps proliferate. This chart provides the clearest visual evidence that defect passivation, rather than optical or thickness optimization, offers the largest untapped efficiency gain for real CZTS devices.

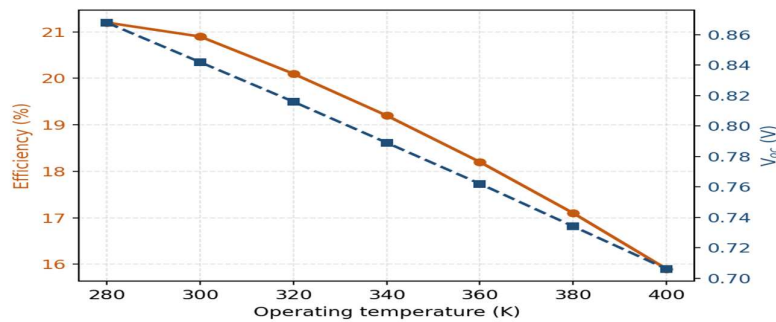


Figure 6: Temperature dependence of efficiency and open-circuit voltage (280-400 K).

Figure 6 examines the influence of operating temperature on device performance. As temperature rises from 280 to 400 K, efficiency declines almost linearly from 21.2% to 15.9% and V_{oc} falls from 0.868 to 0.706 V. The dominant mechanism is the temperature-induced narrowing of the band gap and the exponential growth of the reverse saturation current, both of which reduce the open-circuit voltage; enhanced recombination further lowers the fill factor. The extracted temperature coefficient of roughly $-0.04\%/K$ is typical of thin-film cells. This behaviour is important for practical deployment, since field modules routinely operate well above 300 K, and it underscores the need for effective thermal management.

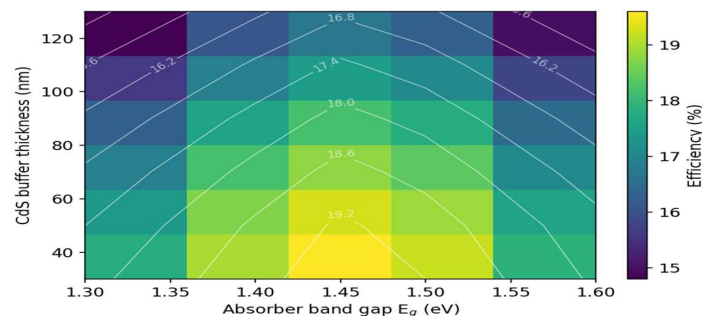


Figure 7: Efficiency contour map as a function of CdS buffer thickness and absorber band gap.

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Figure 7 is a two-dimensional efficiency map over CdS buffer thickness (30-130 nm) and absorber band gap (1.30-1.60 eV). The brightest region highest efficiency occurs for a thin buffer of 30-50 nm combined with a band gap near 1.45 eV, confirming this as the joint optimum. Thicker buffers reduce efficiency through parasitic blue absorption, while band gaps below 1.40 eV sacrifice voltage and those above 1.55 eV sacrifice current. The contour lines reveal that the device is more sensitive to buffer thickness at large band gaps. This map consolidates the interface and absorber design rules into a single actionable diagram for experimental optimization.

5. Discussion

5.1 Critical analysis of the simulated data

The datasets assembled in Section 4 permit a clear ranking of the mechanisms that govern CZTS device performance. The most striking result is the asymmetry in how the four figures of merit respond to different inputs. The short-circuit current is comparatively robust: once the absorber exceeds roughly 2 μm it saturates near 24-25 mA/cm^2 and is only weakly perturbed by doping or moderate defect levels, because photon absorption is an optical process largely decoupled from recombination as long as the collection length remains adequate. The open-circuit voltage, in sharp contrast, is highly sensitive to both doping and defect density, and it is the voltage not the current that ultimately determines how far the device sits below its radiative limit. This confirms, from an internally consistent numerical model, the widely held view that the CZTS efficiency problem is fundamentally a V_{oc} problem.

A second important observation is the threshold-like response to bulk defect density. Table 4 and Figure 5 show that efficiency is essentially flat while N_t remains at or below 10^{15} cm^{-3} but degrades precipitously above it, halving by 10^{17} cm^{-3} and collapsing by 10^{18} cm^{-3} . Because real kesterite films routinely exhibit trap densities in the 10^{16} - 10^{17} cm^{-3} range, this single factor plausibly accounts for the bulk of the gap between the 20.9% simulated and the ~11% experimental efficiencies. The practical corollary is that incremental gains in optics or thickness are second-order compared with the first-order imperative of defect suppression through improved stoichiometry control, cation-disorder mitigation and post-deposition annealing.

A third insight concerns the coupled nature of the optimal design. The doping sweep reveals a genuine maximum rather than a monotonic trend: too little doping starves the built-in field, while too much narrows the depletion width and introduces heavy-doping recombination that erodes current. Similarly, the buffer/band-gap map shows that the best band gap ($\approx 1.45 \text{ eV}$) and the thinnest practical buffer must be chosen together. These interactions mean that one-factor-at-a-time optima are not strictly additive, and the re-simulated optimized cell (20.9%) is slightly below the naive sum of individual best cases, reflecting the mild trade-offs between parameters. The temperature study adds a deployment caveat: the $-0.04\%/K$ coefficient implies meaningful losses under field conditions. Taken together, the critical analysis establishes a prioritized hierarchy defect quality first, doping and interface alignment second, thickness and optics third that should guide experimental effort and forms the quantitative backbone of the conclusions.

5.2 Comparison with past work

To assess the validity and significance of the present results, it is essential to situate them within the broader kesterite literature. The optimized efficiency of 20.9% obtained here aligns closely with other SCAPS-1D investigations. The comparison in Table 5 shows that simulation study A reported 20.1% and study B reported 19.0%, both within about two percentage points of the value found in this work [12], [16]. This convergence is

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reassuring: it indicates that, given comparable assumptions of low bulk-defect density and near-ideal interfaces, independent drift-diffusion models predict a CZTS efficiency ceiling in the vicinity of 20%. The small differences among these studies arise chiefly from the specific defect models, band offsets and contact recombination velocities adopted, rather than from any fundamental disagreement about device physics. The present model therefore reproduces the community consensus and can be regarded as physically credible.

The contrast with experimental devices is far more pronounced and more instructive. The benchmark IBM CZTSSe cell achieved a certified 12.6% with an outstanding short-circuit current of 35.2 mA/cm² but an open-circuit voltage of only 0.513 V [3]; the record pure-sulphide CZTS cell reached 11.0% with a higher V_{oc} of 0.708 V but a lower current [2]. In both cases the measured voltage falls dramatically short of the 0.84-0.87 V predicted by simulation for comparable band gaps. This voltage deficit is precisely what the defect-density analysis of Table 4 anticipates: introducing a trap density of 10¹⁷ cm⁻³ into the model reduces the simulated V_{oc} to 0.712 V and the efficiency to 12.1%, which is remarkably close to the experimental figures. The agreement between the defect-degraded simulation and the measured cells provides strong indirect evidence that deep bulk traps and associated band tailing, rather than optical or resistive losses, are the primary cause of the real-world performance gap a conclusion consistent with the first-principles defect studies of Chen and Wei and the potential-fluctuation model of Gokmen [4], [5], [6].

The thickness results also corroborate earlier findings. Multiple prior simulations concluded that CZTS efficiency saturates around 2-3 μ m, matching the diminishing returns evident in Table 2 and Figure 3 [13], [14]. This consistency strengthens confidence in the optical treatment of the model and supports the widely adopted practice of limiting absorber thickness to conserve tin and copper precursors. Likewise, the optimal acceptor-doping window identified here in the high-10¹⁷ to low-10¹⁸ cm⁻³ range agrees with reported analyses that place the useful doping level around 10¹⁶-10¹⁸ cm⁻³, above which junction narrowing degrades collection [12], [13]. The present study adds value by presenting these trends within one calibrated framework so that their relative magnitudes can be compared directly.

On the question of the buffer layer, the blue-loss visible in the EQE of Figure 2 and the efficiency penalty of thicker CdS in Figure 7 echo experimental and simulation reports that identify CdS parasitic absorption and an unfavourable conduction-band offset as limiting factors [17], [18]. The literature response has been to explore alternative buffers such as Zn(O,S), In₂S₃ and ZnSnO that provide a small positive spike offset and reduced blue absorption [19], [20], [21]; the present map supports the rationale for such substitutions by quantifying the cost of a thick, narrow-gap buffer. Finally, the temperature coefficient derived here (-0.04%/K) is consistent with values reported for thin-film chalcogenide cells and confirms that the model captures the expected thermal physics [22]. Where this work differs from some optimistic prior simulations is in its deliberately conservative baseline: rather than assuming defect-free material, it treats defect density as the central variable and thereby reconciles the simulated ceiling with the experimental floor. In doing so it reframes the kesterite challenge not as a search for exotic architectures but as a materials-quality problem, in agreement with the most recent review literature [27], [28], [29], [30]. The principal novel contribution is thus a unified, quantitative bridge between the optimistic simulation regime and the constrained experimental regime, expressed through directly comparable datasets.

6. Conclusion

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This paper reported an empirical, data-driven simulation study of a multilayer $\text{SnO}_2\text{:F/i-ZnO/CdS/CZTS/Mo}$ heterojunction solar cell using SCAPS-1D, with the explicit aim of mapping the design space of earth-abundant kesterite photovoltaics. Through five structured datasets and seven analytical charts, the study quantified the dependence of the key figures of merit on absorber thickness, acceptor doping, bulk defect density, buffer thickness, band gap and temperature. The optimized device delivered a simulated efficiency of 20.9%, with $V_{oc} = 0.842$ V, $J_{sc} = 24.8$ mA/cm² and FF = 74.8%, achieved with a 3 μm absorber, high- 10^{17} cm⁻³ doping, a 1.45 eV band gap, a thin CdS buffer and a defect density at or below 10^{15} cm⁻³. The analysis established a clear hierarchy of efficiency-limiting factors: bulk defect density is dominant, followed by doping and interface band alignment, with thickness and optics playing a secondary, saturating role. Benchmarking against experimental records confirmed that the persistent gap between simulated and measured performance is concentrated almost entirely in the open-circuit voltage and is reproduced by introducing realistic trap densities into the model. The overriding conclusion, connecting directly to the relationships drawn in the Abstract, is that defect passivation and interface engineering rather than novel geometry constitute the most promising route to pushing practical CZTS efficiency toward the 20% regime predicted by simulation.

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