



## Optimization and Simulation of CIGS Thin-Film Solar Cells Using Cd-Free Buffer Layers

Mohammed Boukhalfa<sup>1</sup>, Mohammed Mostefaoui<sup>2\*</sup>, Roumaissa Zenzen<sup>3</sup>, Abdelkader Azzeddine Bengharbi<sup>4</sup>

<sup>1</sup>Faculty of Science and Technology, Ziane Achour University, 17000, Djelfa, Algeria.

Email: mohamed.boukhalfa@univ-djelfa.dz - ORCID: 0009-0000-5462-698X

<sup>2</sup>Department of Preparatory Classes, Higher School of Saharan Agriculture, Adrar 01000, Algeria,

\* Corresponding Author Email: m.mostefaoui@urms.dz - ORCID: 0000-0002-9364-1530

<sup>3</sup> Laboratory of mechanical engineering, faculty of sciences and technology, university of jijel

Email: roumaissa.zenzen@univ-jijel.dz - ORCID: 0009-0007-8921-9947

<sup>4</sup>Faculty of Technology, Electrical Engineering Department, University of El Oued, Algeria.

Email: bengharbi-aez@univ-eloued.dz - ORCID: 0000-0002-3152-6887

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### Abstract:

In this work, we propose and evaluate four alternative buffer materials  $Zn_2SnO_4$ ,  $ZnS$ ,  $ZrS_xSe_{1-x}$ , and  $SnS_2$  as substitutes for  $CdS$  in CIGS thin-film solar cells. The numerical simulations were performed using SCAPS-1D to study the effect of absorber (CIGS) and buffer layer thickness on the overall photovoltaic performance. The CIGS absorber thickness was varied from  $1 \mu m$  to  $3.5 \mu m$ , while the buffer thickness ranged between  $0.01 \mu m$  and  $0.06 \mu m$ . The results show that increasing the absorber thickness enhances  $V_{oc}$ ,  $J_{sc}$ , and  $\eta$ , with optimal values obtained for  $3.0-3.5 \mu m$ . The influence of buffer thickness was relatively small, with the best performance achieved for  $0.04-0.05 \mu m$ . Among the proposed Cd-free buffer layers,  $ZrS_xSe_{1-x}$  demonstrated the best performance, achieving results nearly identical to those of the conventional  $CdS$  buffer. It exhibited slightly higher  $V_{oc}$  and comparable efficiency ( $\eta \approx 22.4\%$ ), indicating better band alignment and interface properties. Therefore,  $ZrS_xSe_{1-x}$  appears to be a strong environmentally friendly alternative to  $CdS$  for high-efficiency CIGS solar cells. The optimized device structure  $Al/ZnO:Al/ZrS_xSe_{1-x}/CIGS/Mo$  achieved a maximum simulated efficiency of approximately  $22.4\%$ , confirming its potential for next-generation thin-film photovoltaic applications.

## 1. Introduction

Polycrystalline thin-film solar cells based on  $CuInSe_2$  (CIS),  $Cu(In,Ga)Se_2$  (CIGS), and  $CdTe$  are among the most promising alternatives to conventional wafer-based photovoltaic technologies such as Si and GaAs, owing to their high efficiency, long-term stability, and low manufacturing cost [1]. In particular, CIGS and its sulfur-alloyed derivative  $Cu(In,Ga)(S,Se)_2$  (CIGSSe) have attracted significant attention because of their tunable band-gap ( $1.0-1.7$  eV, depending on Ga and S content) and high absorption coefficient ( $\sim 10^5$   $cm^{-1}$ ), which enable efficient light harvesting in sub-micrometer absorber layers [2,3]. Furthermore, CIGS thin films can be deposited on diverse substrates such as glass,

metal foils, and flexible polymers, allowing the fabrication of lightweight, flexible, and low-cost photovoltaic modules [4]. Current CIGS devices have achieved power conversion efficiencies exceeding 20%, placing them among the highest-performing thin-film solar technologies [5]. The standard configuration of a CIGS solar cell consists of a Mo back contact/p-type CIGS absorber/n-type  $CdS$  buffer/i-ZnO/ZnO:Al front contact stack [6]. The  $CdS$  buffer layer, typically deposited by chemical bath deposition (CBD), plays several critical roles:

- It passivates surface defects and grain boundaries on the CIGS absorber,

- Protects the absorber during sputtering of the ZnO window layer, and

Optimizes band alignment at the absorber/buffer interface to facilitate carrier separation and collection[7,8].

Despite these advantages, CdS introduces significant drawbacks. From an environmental perspective, cadmium is toxic and carcinogenic, posing serious health and disposal hazards[9,10]. From an optical

- standpoint, its narrow band-gap ( $E_g \approx 2.4$  eV) results in parasitic absorption losses in the blue and ultraviolet regions, limiting the short-wavelength response and thus overall device performance[11]. Consequently, there is growing interest in developing cadmium-free buffer materials that maintain or exceed the performance of CdS while eliminating its environmental impact[12].

In recent years, a number of wide band-gap, Cd-free materials including ZnS[13], Zn(O,S)[14], ZnSe[15], and  $In_2S_3$  [16] have been investigated as potential replacements for CdS. These materials exhibit larger band-gaps (2.8–3.7 eV), which reduce optical losses, and can provide favorable conduction band alignment with the CIGS absorber. An optimal buffer layer should create a small positive conduction-band offset that effectively blocks holes while promoting electron transport across the junction[16,17]. In this work, we propose and evaluate four alternative buffer materials  $Zn_2SnO_4$ , ZnS,  $ZrS_xSe_{1-x}$ , and  $SnS_2$  as substitutes for CdS in CIGS solar cells. These materials were selected based on their wide band-gaps, chemical stability, and environmental benignity. To assess their suitability, the CIGS solar cell structure was numerically simulated using SCAPS-1D software, which enables detailed modeling of electronic, optical, and interface phenomena in thin-film devices. The simulations aim to analyze the influence of each buffer material on the band alignment, carrier transport, and overall device performance. The ultimate objective of this study is to identify a convenient, non-toxic, and high-performance alternative to CdS that can contribute to the development of sustainable, cadmium-free CIGS solar cells.

## 2. Materials and methodology

### 2.1 Numerical simulation of SCAPS-1D

#### 2.1.1. Device Modelling and Material Parameters

The numerical simulations were conducted using SCAPS-1D (Solar Cell Capacitance Simulator), developed by Dr. Marc Burgelman and his team at

the Department of Electronics and Information Systems, University of Ghent, Belgium[18,19]. SCAPS-1D is a one-dimensional simulation tool widely employed for modeling thin-film solar cells. It solves the coupled Poisson, continuity, and drift diffusion equations under steady-state conditions to describe charge carrier generation, recombination, and transport within multilayer semiconductor devices[15],[20-28].

$$\frac{1}{q} \frac{dJ_n}{dx} = r - g \text{ (for electrons)} \quad (1)$$

$$\frac{1}{q} \frac{dJ_p}{dx} = g - r \text{ (for holes)} \quad (2)$$

Where  $g$  and  $r$  are the generation and recombination rates, respectively, and  $J_n$  and  $J_p$  denote the electron and hole current densities. When both drift and diffusion mechanisms are considered, the current densities can be written as [29-35]:

$$J_p = q\mu_p p \frac{d\phi}{dx} - qD_p \frac{dp}{dx} \quad (3)$$

$$J_n = q\mu_n n \frac{d\phi}{dx} - qD_n \frac{dn}{dx} \quad (4)$$

Where  $\mu_p$  and  $\mu_n$  are the mobilities of holes and electrons,  $D_p$  and  $D_n$  are their corresponding diffusion coefficients,  $p$  and  $n$  are the carrier concentrations,  $q$  is the elementary charge, and  $\phi$  is the electrostatic potential. The relationship between charge density  $\rho$  and electrostatic potential  $\phi(x)$  is governed by the Poisson equation [35-40]:

$$\frac{d^2\phi(x)}{dx^2} = -\frac{\rho}{\epsilon} \quad (5)$$

Where:

$$\rho = q(p - n + N_D^+ - N_A^-) \quad (6)$$

Substituting Eq. (6) into Eq. (5) yields:

$$\frac{d^2\phi(x)}{dx^2} = -\frac{q}{\epsilon_0 \epsilon_r} (p - n + N_D^+ - N_A^-) \quad (7)$$

Here,  $\epsilon_0$  and  $\epsilon_r$  denote the vacuum and relative permittivities, respectively;  $N_D^+$  and  $N_A^-$  represent the concentrations of ionized donors and acceptors. Together, these equations form the physical foundation of the SCAPS-1D model, describing the balance between carrier transport, electrostatic potential distribution, and recombination mechanisms within the simulated solar cell structure.

#### 2.1.2. CIGS solar cell structure

The simulated architecture of the CIGS solar cell consists of a multilayer heterojunction stack arranged as Al / ZnO:Al / Buffer Layer / CIGS / Back Contact, which represents a conventional and well-established thin-film CIGS photovoltaic device configuration. Each layer in this structure fulfills a specific electrical and optical function that is essential for efficient photovoltaic operation.

The Aluminum (Al) layer is employed as the front metallic contact, ensuring efficient extraction and collection of photogenerated charge carriers. Due to its low electrical resistivity and good compatibility with transparent conductive oxides, Al provides minimal series resistance and contributes to reduced ohmic losses in the device.

The Al-doped Zinc Oxide (ZnO:Al) layer serves as the transparent conductive oxide (TCO). This layer plays a dual role by allowing maximum transmission of incident solar radiation into the absorber layer while simultaneously acting as a highly conductive pathway for electron transport toward the external circuit. Aluminum doping significantly enhances the electrical conductivity of ZnO without compromising its high optical transparency in the visible spectrum, thereby improving the overall current collection efficiency.

The buffer layer is a thin n-type semiconductor positioned between the TCO and the absorber. Its primary function is to form a high-quality p-n heterojunction with the p-type CIGS absorber, enabling effective separation of photogenerated electron-hole pairs. Additionally, the buffer layer improves band alignment at the interface, reduces interface defect density, and suppresses carrier recombination losses. Although cadmium sulfide (CdS) is the most widely used buffer material due to its favorable electronic properties and interface quality, alternative cadmium-free buffer layers such as Zn<sub>2</sub>SnO<sub>4</sub>, ZnS, ZrS<sub>x</sub>Se<sub>1-x</sub>, and SnS<sub>2</sub> have been investigated to address environmental and toxicity concerns while maintaining high device performance.

The CIGS (Cu(In,Ga)Se<sub>2</sub>) layer acts as the p-type absorber and is the core photoactive region of the solar cell. Owing to its high optical absorption coefficient, a relatively thin CIGS layer is sufficient to absorb the majority of the incident sunlight and generate electron-hole pairs. One of the key advantages of CIGS is its tunable bandgap, which can be adjusted from approximately 1.0 to 1.7 eV by varying the Ga/(In+Ga) ratio. This tunability allows optimization of the absorber for enhanced open-circuit voltage and overall power conversion efficiency.

The back contact layer, typically molybdenum (Mo) or, in the present simulation, platinum (Pt), provides an ohmic contact with the CIGS absorber and ensures efficient hole collection. This layer also offers good mechanical stability and adhesion to the substrate, which is crucial for device reliability and fabrication compatibility.

In this work, the simulated CIGS solar cell structure is defined as Al / ZnO:Al / CdS / CIGS / Pt, as illustrated in Figure 1. All simulations were performed at a standard operating temperature of 300 K, assuming constant carrier mobility across all layers. The electrical and optical material parameters employed in the simulations were extracted from well-established and reliable literature sources, and a detailed summary of these parameters is provided in Table 1.

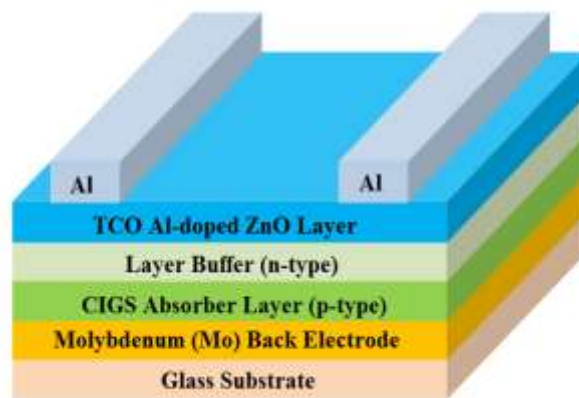


Figure 1. The general structure of a CIGS thin film solar cell

Table 1: Summary of initial parameters set for the simulation of CIGS solar cells [41-49].

Material properties	CIGS	CdS	Zn <sub>2</sub> SnO <sub>4</sub>	ZnS	ZnO	ZrS <sub>x</sub> Se <sub>2-x</sub>
Thickness (μm)	Variable	0.1	0.1	0.1	0.1	0.2
Bandgap (E <sub>g</sub> )	1.100	2.4	3.3500	3.5	3.3	1.3
Electron affinity χ (eV)	4.500	2.4	4.5000	4.5	4.5	4.7
Dielectric permittivity ε	13.600	10	9.000	10	9.00	16.4
CB density of state	2.200E+18	2.200E+18	2.200E+18	1.500E+18	2.200E+18	2.200E+18
VB density of state	1.800E+19	1.800E+19	1.800E+19	1.800E+18	1.800E+19	1.800E+19

Electron thermal velocity	1.000E + 7	1.000E + 7	1.000E + 7	1.000E + 7	1.000E + 7	1.000E + 7
Hole thermal velocity	1.000E + 7	1.000E + 7	1.000E + 7	1.000E + 7	1.000E + 7	1.000E + 7
Electron mobility	1.00E+2	1.00E+2	3.200E + 1	50	1.00E + 2	2300
Hole mobility	2.50E+1	2.50E+1	3.000E + 0	20	2.00E + 1	1300
Donor density	1.00E+18	1.00E+18	1.000E + 19	1.00E+18	1.00E+18	1.00E+18
Acceptor density	0.00E+0	0.00E+0	0.000E + 0	0.00E+0	1.00E+5	0.00E+0
Absorption coefficient	SCAPS value	SCAPS value	SCAPS value	SCAPS value	SCAPS value	SCAPS value

### 3. Result and discussion

#### 3.1 Simulation of CIGS–ZnO(Al) solar cells with Different Buffer Layers :

We initially studied the buffer layer to evaluate its influence on the overall performance of the CIGS (Cu(In,Ga)Se<sub>2</sub>) thin-film solar cell. The buffer layer plays a crucial role in forming the p–n junction between the CIGS absorber (p-type) and the ZnO:Al window layer (n-type), ensuring efficient charge separation and transport. To investigate this effect, several buffer materials were simulated using the Solar Cell Capacitance Simulator (SCAPS) software, including CdS, ZnS, SnS<sub>2</sub>, Zn<sub>2</sub>SnO<sub>4</sub>, and ZrS<sub>x</sub>Se<sub>2-x</sub>. Each material was evaluated under the same device structure (Al/ZnO:Al/Buffer/CIGS/Mo) and standard test conditions (AM 1.5G, 1000 W/m<sup>2</sup>, 300 K). The results showed that all studied structures exhibited high photovoltaic performance, with conversion efficiencies ranging from 21.5% to 22.1%. Among the investigated materials, CdS, SnS<sub>2</sub>, and ZrS<sub>x</sub>Se<sub>2-x</sub> provided the best results, reaching efficiencies around 22.1%, due to their favorable band alignment and low interface recombination with the CIGS absorber. The Zn<sub>2</sub>SnO<sub>4</sub> and ZnS layers also demonstrated comparable performance ( $\eta \approx 21.6\%$ ) and are considered promising Cd-free alternatives that combine high transparency with good electrical compatibility. These findings confirm that proper buffer layer selection and optimization are essential to achieving high-efficiency, environmentally friendly CIGS-based thin -film solar cells. The simulation results indicate that all CIGS-based solar cells exhibit high efficiencies (21.6–22.1%), with slight variations in the open-circuit voltage (Voc) and short-circuit current density (Jsc). Among the studied buffer materials, CdS, SnS<sub>2</sub>, and ZrS<sub>x</sub>Se<sub>2-x</sub> achieved the highest efficiencies (~22.1%), showing optimal band alignment and low interface recombination. Meanwhile, Zn<sub>2</sub>SnO<sub>4</sub> and ZnS demonstrate competitive performance and are considered promising cadmium-free alternatives due to their excellent transparency and environmental

safety. The J–V characteristics (left) show that all simulated structures exhibit nearly identical diode behavior with high short-circuit current density ( $J_{sc} \approx 38\text{--}39 \text{ mA/cm}^2$ ) and open-circuit voltage ( $V_{oc} \approx 0.676 \text{ V}$ ). The QE spectra (right) confirm a strong photoresponse in the wavelength range 400–1000 nm, indicating efficient photon absorption by the CIGS absorber layer. Among the studied buffer materials, CdS, SnS<sub>2</sub>, and ZrS<sub>x</sub>Se<sub>2-x</sub> show slightly higher quantum efficiency across the visible spectrum, consistent with their higher conversion efficiencies (~22%). These results confirm the excellent optical and electrical performance of the CIGS–ZnO(Al) structures with different buffer layers.

**Table 2 :** Simulated performance parameters of CIGS–ZnO(Al) solar cells with different buffer layers

Buffer Layer	Voc (V)	Jsc (mA/cm <sup>2</sup> )	FF (%)	$\eta$ (%)
CdS	0.6764	39.20	83.37	22.10
SnS <sub>2</sub>	0.6765	39.19	83.32	22.09
Zn <sub>2</sub> SnO <sub>4</sub>	0.6758	38.36	83.34	21.60
ZnS	0.6758	38.35	83.33	21.59
ZrS <sub>x</sub> Se <sub>2-x</sub>	0.6769	39.23	83.23	22.10

**Table 3.** Effect of Absorber Layer Thickness on CIGS Solar Cell Performance for CdS (0.05  $\mu\text{m}$ ) Buffer.

Absorber Thickness ( $\mu\text{m}$ )	Voc (V)	Jsc (mA/cm <sup>2</sup> )	FF (%)	$\eta$ (%)
1.0	0.6657	37.67	83.00	20.81
1.5	0.6697	38.43	83.14	21.40
2.0	0.6732	38.88	83.27	21.80
2.5	0.6764	39.19	83.37	22.10
3.0	0.6793	39.44	83.44	22.36
3.5	0.6817	39.65	83.54	22.58

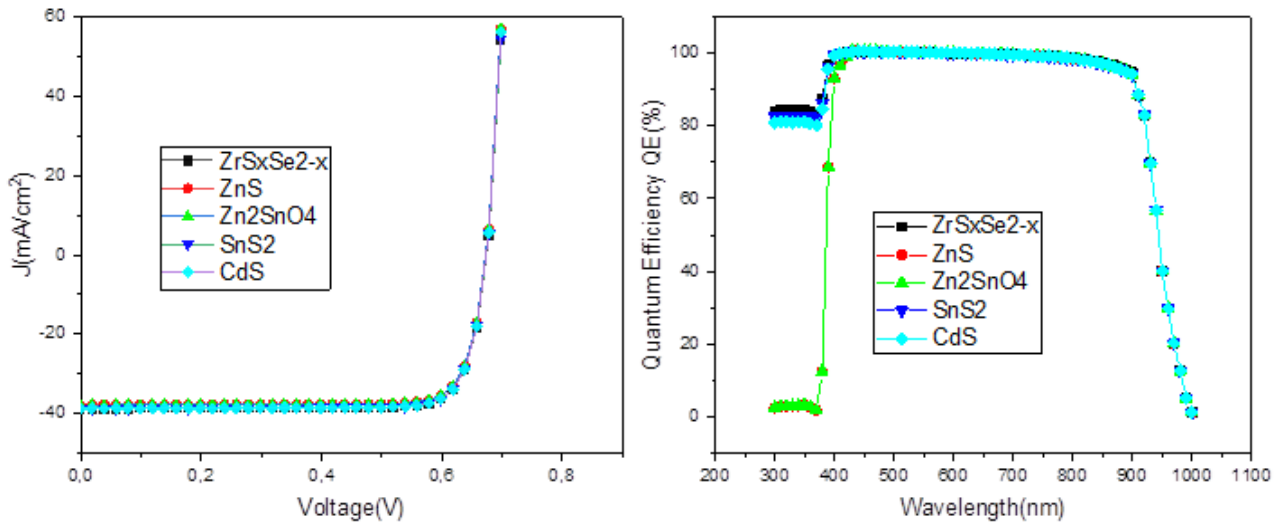


Figure 2. J–V characteristics and Quantum Efficiency (QE) curves for CIGS solar cells with different buffer layers (CdS, SnS<sub>2</sub>, Zn<sub>2</sub>SnO<sub>4</sub>, ZnS, and ZrS<sub>x</sub>Se<sub>2-x</sub>).

### 3.2 Effect of Absorber and Buffer Layer Thickness on CIGS Solar Cell Performance

#### a. Effect of Absorber Layer Thickness:

To investigate the influence of absorber thickness on device performance, the CIGS absorber layer thickness was varied from 1 μm to 3.5 μm, while the buffer layer (CdS or ZrS<sub>x</sub>Se<sub>2-x</sub>) was kept constant at 0.05 μm. The corresponding photovoltaic parameters open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and efficiency (η) are summarized in Table 3 and Table 4.

Table 4. Effect of Absorber Layer Thickness on CIGS Solar Cell Performance for ZrS<sub>x</sub>Se<sub>2-x</sub> (0.05 μm) Buffer.

Absorber Layer (μm)	Voc (V)	Jsc (mA/cm <sup>2</sup> )	FF (%)	η (%)
1	0.666	37.76	82.85	20.85
1.5	0.670	38.48	83.00	21.41
2	0.6737	38.91	83.13	21.80
2.5	0.6769	39.22	83.23	22.10
3	0.6798	39.46	83.31	22.35
3.5	0.6820	39.66	83.43	22.57

As shown in Tables 3 and 4, the photovoltaic parameters (Voc, Jsc, and η) steadily improve as the CIGS absorber thickness increases from 1 μm to 3.5 μm. This improvement is primarily due to enhanced photon absorption and increased carrier generation in thicker absorber layers. However, beyond 3 μm, the improvement becomes marginal since most of the incident light is already absorbed within the layer, and excessive thickness may increase recombination losses. The maximum efficiency (η ≈

22.6%) is obtained at an absorber thickness of 3.5 μm for both CdS and ZrS<sub>x</sub>Se<sub>2-x</sub> based structures. The solar cell employing ZrS<sub>x</sub>Se<sub>2-x</sub> as a buffer layer exhibits slightly higher Voc and η, suggesting improved band alignment and interface quality compared to CdS. Therefore, an absorber thickness in the range of 3–3.5 μm is considered optimal for achieving high-efficiency CIGS solar cells.

#### b. Effect of Buffer Layer Thickness

To examine the influence of the buffer layer thickness on the photovoltaic performance of CIGS-based solar cells, the CIGS absorber layer thickness was fixed at 2.5 μm, while the buffer layer thickness was varied between 0.01 μm and 0.06 μm. The corresponding values of open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and conversion efficiency (η) are summarized in Table 5 and Table 6 for CdS and ZrS<sub>x</sub>Se<sub>2-x</sub> buffer layers, respectively. As seen in Tables 5 and 6, changing the buffer layer thickness from 0.01 μm to 0.06 μm has only a minor impact on the photovoltaic

Table 5. Effect of Buffer Layer Thickness on CIGS Solar Cell Performance for CdS Buffer (2.5 μm Absorber)

Buffer Thickness (μm)	Voc (V)	Jsc (mA/cm <sup>2</sup> )	FF (%)	η (%)
0.01	0.6764	39.22	83.33	22.11
0.02	0.6764	39.21	83.36	22.11
0.03	0.6764	39.20	83.36	22.11
0.04	0.6764	39.20	83.37	22.10
0.05	0.676	39.19	83.37	22.10
0.06	0.6764	39.19	83.37	22.10

**Table 6.** Effect of Buffer Layer Thickness on CIGS Solar Cell Performance for  $ZrS_xSe_{2-x}$  Buffer ( $2.5 \mu m$  Absorber).

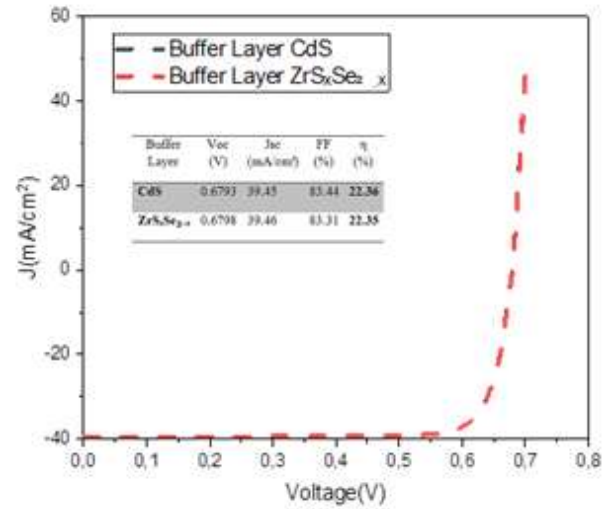
Buffer Thickness ( $\mu m$ )	Voc (V)	Jsc ( $mA/cm^2$ )	FF (%)	$\eta$ (%)
0.01	0.6767	39.17	83.06	22.02
0.02	0.6767	39.17	83.08	22.03
0.03	0.6768	39.19	83.12	22.05
0.04	0.6768	39.20	83.16	22.6
0.05	0.6768	39.21	83.20	22.08
0.06	0.6769	39.22	83.23	22.10

parameters. The values of Voc, Jsc, and FF remain nearly constant, while the efficiency ( $\eta$ ) shows a small variation around 22.1%. The optimal buffer thickness lies between  $0.04 \mu m$  and  $0.05 \mu m$ , where the device achieves stable and maximum efficiency. Thinner buffer layers ( $<0.02 \mu m$ ) can cause incomplete junction formation and higher leakage currents, whereas thicker layers ( $>0.06 \mu m$ ) tend to absorb part of the incident light, leading to a slight decrease in Jsc. When comparing both materials, the cell with  $ZrS_xSe_{2-x}$  buffer demonstrates slightly higher Voc and  $\eta$  values than the CdS-based cell, confirming better band alignment and reduced interface recombination. Therefore, a buffer thickness of  $0.04\text{--}0.05 \mu m$  combined with a  $2.5 \mu m$  CIGS absorber layer provides the optimal configuration for achieving high-efficiency and environmentally friendly CIGS solar cells.

### 3.3 Optimal Solar Cell Parameters

The best configuration of the simulated CIGS solar cell corresponds to an absorber thickness of  $3.5 \mu m$  and a buffer thickness of  $0.05 \mu m$ . The deduced photovoltaic parameters from the calculated J–V (current–voltage) characteristics for both CdS and  $ZrS_xSe_{2-x}$  buffer layers are summarized below. The simulation results show that both buffer materials lead to nearly identical photovoltaic performance under optimized conditions. The CdS-based cell exhibits a slightly higher fill factor (FF), resulting in a marginally higher efficiency of 22.36%. The  $ZrS_xSe_{2-x}$ -based cell, however, shows a slightly higher Voc, indicating improved band alignment and potentially lower recombination losses at the interface. Although the efficiency difference is minimal,  $ZrS_xSe_{2-x}$  offers an environmentally friendly and cadmium-free alternative to CdS, while maintaining comparable device performance. Therefore,  $ZrS_xSe_{2-x}$  can be considered a promising

substitute for CdS in high-efficiency CIGS thin-film solar cells.



**Figure 3.** J–V characteristics of optimized CIGS–ZnO(Al) solar cell structures with different buffer layers.

### 4. Conclusion

In this study, the performance of CIGS thin-film solar cells was numerically investigated using the SCAPS-1D simulation program. The effects of both the absorber (CIGS) and buffer (CdS and  $ZrS_xSe_{2-x}$ ) layer thicknesses on the photovoltaic parameters were systematically analyzed. The results demonstrated that increasing the CIGS absorber thickness from  $1 \mu m$  to  $3.5 \mu m$  enhances the device efficiency due to improved photon absorption and carrier generation. However, beyond  $3 \mu m$ , the improvement becomes marginal as most of the incident light is already absorbed, and thicker layers may induce additional recombination. The optimal absorber thickness was found to be between  $3.0 \mu m$  and  $3.5 \mu m$ , where the maximum efficiency of approximately 22.6% was achieved. Similarly, the buffer layer thickness showed only a minor influence on device performance, with optimal results obtained for thicknesses between  $0.04 \mu m$  and  $0.05 \mu m$ . Both buffer materials exhibited comparable performance, but the  $ZrS_xSe_{2-x}$  layer provided slightly higher Voc and overall stability, highlighting its potential as a Cd-free and environmentally friendly alternative to conventional CdS. In conclusion, the optimized configuration consisting of a CIGS absorber ( $3.5 \mu m$ ) and a  $ZrS_xSe_{2-x}$  buffer layer ( $0.05 \mu m$ ) yields the best balance between light absorption, carrier transport, and junction quality, resulting in an efficiency of about 22.4%. These findings confirm the strong potential of CIGS/ $ZrS_xSe_{2-x}$ -based solar cells for the development of high-performance, sustainable photovoltaic devices.

## 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
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