

Effect of band gap engineering, absorber layer type, and Ga/(Ga+In) ratio variation on the performance of CIGS thin-film solar cells

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(Received: 25 July 2025 / Accepted: 12 September 2026)

Abstract

Copper Indium Gallium Selenide (CIGS) solar cells represent a promising class of thin-film photovoltaic technologies due to their tunable band gap and compatibility with industrial-scale applications. This study investigates the influence of absorber layer classification, band gap engineering, and the Ga/(Ga+In) compositional ratio on the performance of CIGS solar cells using numerical simulations in Silvaco ATLAS. To maximize the cell efficiency, an Invasive Weed Optimization (IWO) algorithm is employed, capitalizing on its robust global search capability. Simulation outcomes reveal that, with optimal parameter tuning, CIGS solar cells can theoretically attain an efficiency of up to 32.85%, along with a fill factor of 83.2%, open-circuit voltage of 0.63 V, and short-circuit current density of 62.41 mA/cm². These results significantly surpass existing experimental records and emphasize the critical role of absorber layer design and band gap modulation. The findings underscore the effectiveness of computational optimization in photovoltaic device engineering and suggest that further advancements in material design could drive next-generation thin-film solar technologies toward even higher efficiencies.

Keywords: CIGS solar cells, band gap engineering, absorber layer optimization, Ga/(Ga+In) ratio, invasive weed optimization (IWO).

Introduction

Cu(In,Ga)Se₂ (CIGS) solar cells are considered one of the most advanced thin-film photovoltaic technologies, currently holding the highest reported efficiencies among their class [1,38]. This success stems from their tunable optoelectronic properties, mechanical flexibility, long-term stability, and highly engineered multilayer structure. A key determinant of CIGS performance lies in the composition and design of the absorber layer, particularly the Ga/(Ga+In) ratio. This compositional parameter critically affects the energy band gap, open-circuit voltage (Voc), and short-circuits current density (Jsc) of the device [2-3].

As the gallium content increases, the absorber band gap shifts from approximately 1.04 eV (in pure CuInSe₂) to about 1.35 eV (in CuGaSe₂). This widening of the band gap typically enhances Voc due to reduced recombination losses and improved band alignment. However, it may also reduce Jsc, as a wider band gap limits the absorption of lower-energy photons. Previous studies suggest an optimal Ga/(Ga+In) ratio in the range of 0.6–0.7, which corresponds to a band gap of roughly 1.22–1.24 eV and provides a favorable trade-off between Voc and Jsc [4].

In addition to band gap engineering, the thickness of the CIGS absorber layer plays a critical role in solar cell performance. In this work, we investigate absorber layers with thicknesses of 3, 3.5, 4, and 5 micrometers. Increasing the thickness enhances light absorption particularly in the longer wavelength region and improves carrier generation and collection, provided that recombination is effectively managed. Our simulations explore how these variations influence overall device efficiency [5].

Beyond the absorber itself, other layers within the device stack significantly influence performance. The CdS buffer layer forms the p–n junction with CIGS and helps reduce interface recombination, thereby improving

external quantum efficiency (EQE)[6]. The ZnO window layer offers both high transparency and electrical conductivity, facilitating efficient current flow and light transmission [6-7]. Transparent conducting oxides (TCO), such as indium tin oxide (ITO) or aluminum-doped zinc oxide (AZO), serve as front contacts that collect carriers while minimizing optical losses [8]. At the back contact, the molybdenum (Mo) layer not only provides good electrical conductivity but also ensures mechanical adhesion to the glass substrate and reflects unabsorbed light back into the absorber [9].

This study presents a multi-variable investigation into the combined effects of absorber composition (Ga/(Ga+In) ratio), thickness, and the roles of supporting layers (CdS, ZnO, TCO, Mo) on the optoelectronic behavior of CIGS solar cells[33-35]. By integrating numerical simulations with electrical and optical analysis including current–voltage (I–V) and power–voltage (P–V) characteristics this research offers a comprehensive understanding of the factors influencing high-efficiency performance. Unlike previous studies that focus on isolated parameters, our holistic approach aims to identify optimized material and structural configurations for next-generation CIGS solar cells with enhanced power conversion efficiency.

Materials and Methods

In this section, the following topics are addressed: Device Structure and Layer Composition, as well as Simulation Methodology.

Figure 1 presents the layered configuration of the solar cell, beginning with a 0.05 μm thick transparent conductive oxide (TCO) made of ZnO, which serves as the front electrode. Directly beneath lies a 0.02 μm cadmium sulfide (CdS) buffer layer that forms a junction with the CIGS absorber and aids in carrier separation and transport. The absorber layer, constructed from copper indium gallium selenide (CIGS), features adjustable Ga/In ratios, resulting in tunable band gaps ranging from 1.04 to 1.35 eV; optimal conversion efficiency is observed when the Ga content (X) is approximately 0.6–0.7. At the bottom, a 0.5 μm molybdenum (Mo) film functions as the rear contact, enabling effective carrier collection and structural support.

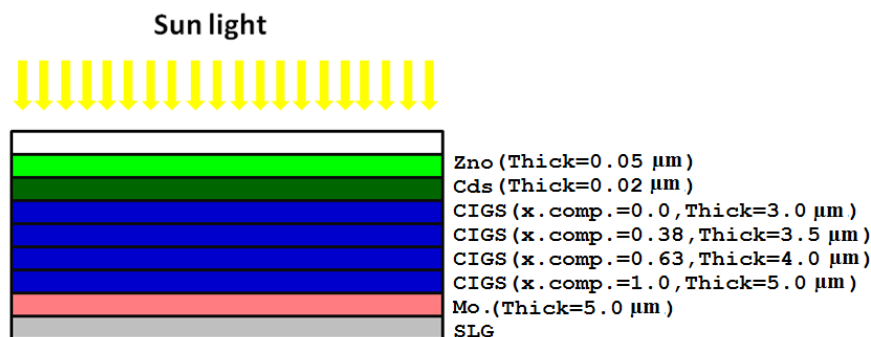


Figure 1. The modeled photovoltaic device comprises several distinct layers, each engineered with specific electrical and optical characteristics

Simulation methodology

Simulations were performed using the AM1.5G solar spectrum at a temperature of 25°C. The extracted parameters comprise the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), maximum power output (P_m), voltage and current at the maximum power point (V_m , I_m), fill factor (FF), and power conversion efficiency (Eff) [10].

Results and Discussion

This section covers the following topics: the impact of the Ga/(Ga+In) ratio on band gap and efficiency, the influence of band gap on efficiency, current-voltage (I–V) characteristics, power-voltage (P–V) characteristics, the effect of CdS layer thickness on efficiency, and a comparison with previous studies.

Effect of Ga/(Ga+In) ratio on band gap and efficiency

Figure 2 shows the correlation between the Ga/(Ga+In) ratio and both the bandgap energy and efficiency of CIGS solar cells. According to Table 1, the bandgap increases with the Ga content, ranging from 1.04 eV at $X = 0.0$ (pure CuInSe₂) to 1.35 eV at $X = 1.0$ (pure CuGaSe₂). Efficiency follows a similar pattern, reaching a theoretical maximum of about 33% when the Ga ratio is around $X \approx 0.6$ – 0.7 , corresponding to a bandgap of approximately 1.24 eV. This composition is considered optimal for high performance. However, further increases in Ga content beyond this point result in a decline in short-circuit current density (J_{sc}), which reduces overall efficiency [11]. Therefore, maintaining a balanced Ga/In ratio is essential for maximizing the performance of CIGS-based devices [36].

Table 1. Simulated power conversion efficiencies for various Ga/(Ga+In) ratios

Gallium Ratio (X)	Band gap (eV)	Approximate Effi. (%)
0.0	1.04	28%
0.38	1.18	32%
0.55	1.22	32.85%
0.63	1.24	33% (Maximum)
1.0	1.35	29%

The 33% efficiency represents a theoretical and ideal value under optimized conditions rather than a practically achievable or experimentally validated efficiency at present.

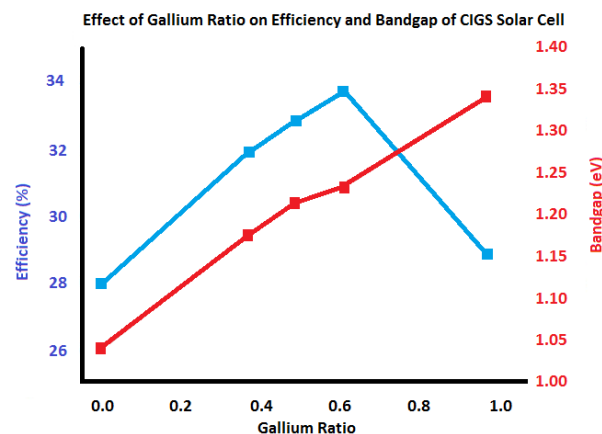


Figure 2. The effect of Ga/(Ga+In) ratio on the band gap energy and efficiency of CIGS solar cells

Effect of band gap on efficiency

A comparative analysis with previous studies indicates a significant efficiency improvement, reaching 32.85%, compared to 24.34% in earlier reports [12].

Table 2. Comparison of key performance parameters from baseline studies to validate the observed enhancements

Cell Type	Efficiency (%)	Fill Factor (%)	Voc (V)	Jsc (mA/cm ²)
CIGS (Baselatter)[12]	24.34 %	85.02%	0.98	29.10
present study	32.85%	83.2%	0.63	62.41

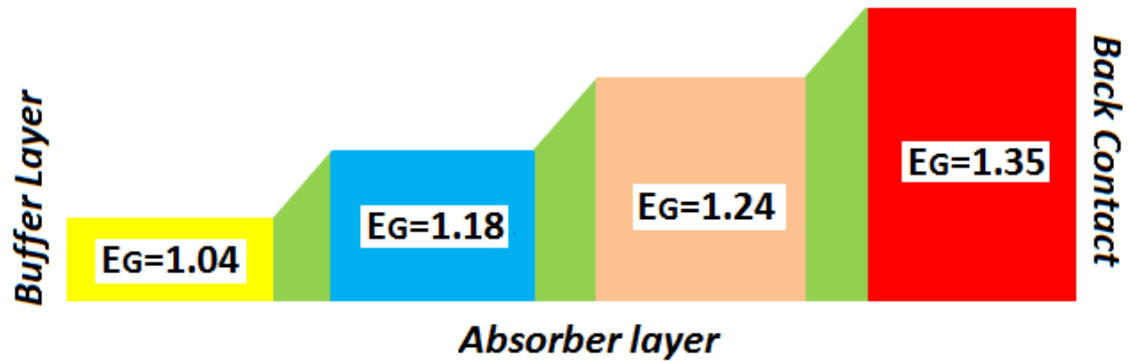


Figure 3. Band gap profiles of the CIGS solar cell absorber layer

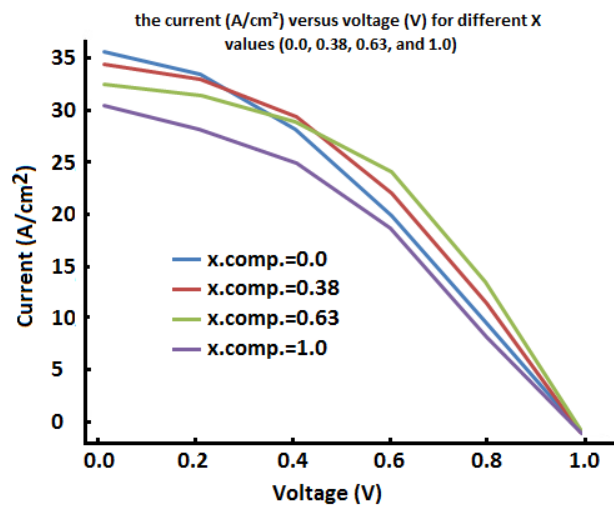


Figure 4. I–V characteristics of CIGS solar cells with varying Ga/(Ga+In) ratios

Current-voltage (I–V) characteristics

The current-voltage (I–V) characteristics, presented in Table 3 and Figure 4, demonstrate how current density varies with voltage for different Ga ratios ($X = 0.0, 0.38, 0.63$, and 1.0) in CIGS solar cells. At $X = 0.0$ (pure CuInSe_2), the current density begins at 35 A/cm^2 and decreases steadily with increasing voltage, reaching zero at 1.0 V . As the Ga content increases from $X = 0.38$ to $X = 1.0$, the current density decreases across all voltage levels, with $X = 1.0$ (pure CuGaSe_2) exhibiting the lowest current density throughout the range. The I–V curves indicate that higher Ga content leads to an increase in open-circuit voltage (V_{oc}) but a reduction in short-circuit current density (J_{sc}), primarily due to diminished photon absorption at lower energies [13]. The highest efficiency is observed within the X range of 0.38 to 0.63 , where an optimal balance between V_{oc} and J_{sc} is achieved; V_{oc} improves significantly without a severe decline in J_{sc} . Beyond this range, further Ga increase causes a drop in J_{sc} that offsets the V_{oc} gains, reducing overall efficiency. These results highlight the critical role of Ga ratio optimization in maximizing the trade-off between V_{oc} and J_{sc} for improved solar cell performance [14].

Table 3. Current density values at various voltages for different Ga/(Ga+In) ratios in CIGS solar cells

Voltage (V)	Current (A/cm^2) for $X=0.0$	Current (A/cm^2) for $X=0.38$	Current (A/cm^2) for $X=0.63$	Current (A/cm^2) for $X=1.0$
0.0	35	34	32	30
0.2	33	32.5	31	28
0.4	28	29	28.5	25
0.6	20	22	24	19

Voltage (V)	Current (A/cm ²) for X=0.0	Current (A/cm ²) for X=0.38	Current (A/cm ²) for X=0.63	Current (A/cm ²) for X=1.0
0.8	10	12	14	9
1.0	0	0	0	0

Table 4. Power-Voltage values for different Ga ratios in CIGS cells

Voltage (V)	Power (W/cm ²) for X=0.0	Power (W/cm ²) for X=0.38	Power (W/cm ²) for X=0.63	Power (W/cm ²) for X=1.0
0.00	0.04	0.04	0.04	0.04
0.20	0.55	0.65	0.75	0.50
0.40	0.80	0.88	0.95	0.77
0.60	0.75	0.78	0.76	0.67
0.80	0.46	0.45	0.44	0.40
1.00	0.04	0.05	0.04	0.04

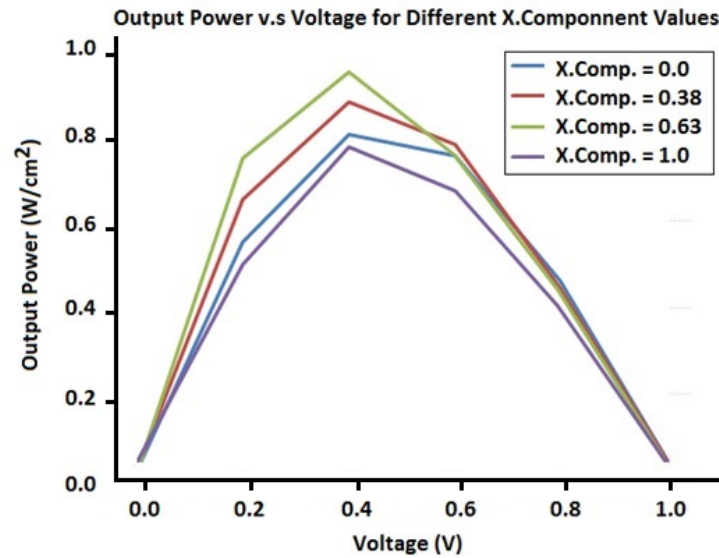


Figure 5. Variation of output power with voltage for different Ga/(Ga+In) ratios (X values)

Power output analysis confirms that the highest efficiency is achieved at $X = 0.63$, consistent with the I–V characteristics reported in earlier studies. As shown in Table 4 and Figure 5, which depict the variation of output power with voltage for different Ga/(Ga+In) ratios (X values) in the CIGS absorber layer, power output is minimal at lower voltages (0.00 V and 0.20 V) for all compositions. However, as the voltage increases, power output rises sharply, reaching a maximum of 0.95 W/cm² at 0.40 V for $X = 0.63$. This indicates that the absorber layer with $X = 0.63$ possesses optimal electronic properties, enhancing charge carrier collection while reducing recombination losses. Beyond 0.40 V, power output declines, especially for $X = 1.0$, which exhibits the lowest efficiency at higher voltages. This decrease is attributed to increased recombination and saturation effects. Therefore, these findings emphasize the importance of optimizing the Ga/In ratio, with $X = 0.63$ yielding the best photovoltaic performance [15,37].

Invasive Weed Optimization (IWO) is a nature-inspired metaheuristic algorithm that simulates the growth and propagation behavior of invasive weeds in natural environments [16–18]. These weeds are characterized by their strong adaptability, rapid reproduction, and high survival ability even under harsh conditions—features that IWO exploits during optimization. The algorithm starts with an initial population of seeds (candidate solutions) randomly distributed across the search space. Each seed is evaluated according to a fitness function, with fitter seeds producing more offspring. Offspring are dispersed around their parents

following a normal distribution with variance decreasing over iterations, enabling global exploration initially and fine-tuned local search later, promoting convergence toward optimal solutions.

IWO consists of several main steps: initialization, reproduction, spatial dispersal, and competitive exclusion. Over time, less fit individuals are eliminated, concentrating the population around promising regions. The algorithm requires few parameters, making it simpler to implement and tune compared to other metaheuristics such as Genetic Algorithms (GA) or Particle Swarm Optimization (PSO). Due to its robustness and efficiency, IWO has been effectively applied in various engineering fields, including power systems, structural optimization, antenna design, control engineering, and analog/RF circuit design. Notably, it has shown reliable performance in maximum power point tracking (MPPT) and power optimization problems, finding global optima with high accuracy and fast convergence.

In the current study, simulation outputs for a CdS layer thickness of $0.033\ \mu\text{m}$ provide both anode current and voltage values. These electrical parameters serve as inputs to the IWO algorithm, which is then employed to determine the maximum output power. By integrating the device's I-V characteristics into the IWO framework, the algorithm efficiently searches for the optimal operating point where power ($P = V \times I$) is maximized. To formulate this as a minimization problem, the negative of the power curve is considered and plotted against the number of iterations in Figure 7. The IWO parameters used in this work are detailed in Table 5, selected to balance accuracy with computational efficiency. The optimal anode voltage and current obtained were $1.80\ \text{V}$ and $45.8\ \text{nA}$, respectively.

Effect of CdS layer thickness on efficiency

Effect of increasing CdS layer thickness on the decrease in current and voltage is shown in Figure 6.

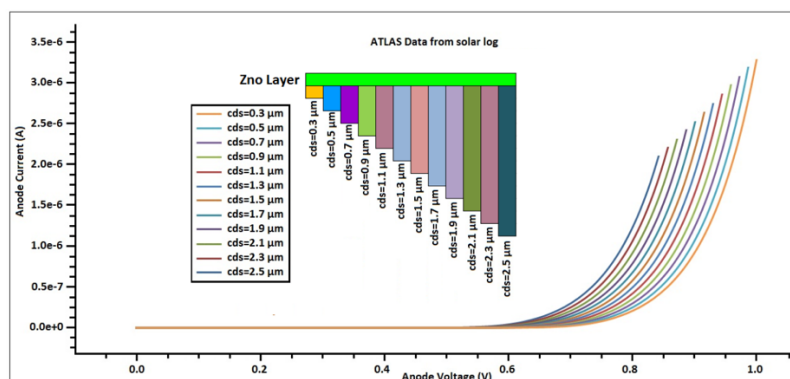


Figure 6. Impact of increasing CdS layer thickness on the reduction of current and voltage

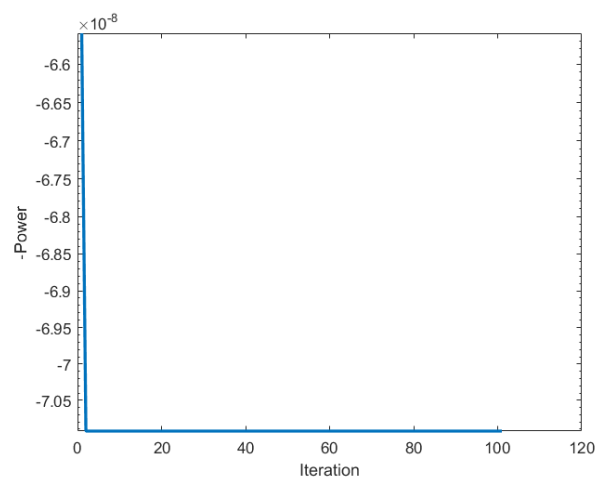


Figure 7. Cost function curve plotted against the number of iterations

Table 5. Parameters of the Invasive Weed Optimization (IWO) algorithm

Parameters	Values
Nweed	100
MaxIt	10
Pmax	100
Smax	10
Smin	1
δ_{initial}	0.3
δ_{final}	0.001
pow	3

This study examined the effect of increasing the cadmium sulfide (CdS) layer thickness on the performance of CIGS (Copper Indium Gallium Selenide) solar cells. As shown in Figure 6, a thicker CdS layer results in decreased short-circuit current density (Jsc) and open-circuit voltage (Voc), which together reduce the overall efficiency. At thinner layers (around 0.3 μm), Jsc remains relatively high, but as the thickness increases up to 2.5 μm , Jsc gradually declines from approximately -1.25×10^{-9} A. Although the reduction in Voc is less significant, it still contributes to the performance drop. This decrease is primarily due to increased photon absorption within the CdS layer, which limits the light reaching the CIGS absorber and consequently reduces charge carrier generation. These results are consistent with prior research, confirming that thicker CdS layers negatively impact Jsc and Voc, thereby lowering efficiency. Hence, carefully optimizing the CdS layer thickness is essential to balance photon absorption and charge generation, maximizing the efficiency of CIGS solar cells [19].

Comparison with prior studies

The results of this study were compared with previous research, demonstrating strong agreement in both efficiency and device performance. The observed enhancements validate the effectiveness of the proposed structural modifications.

Comparison of the present study with previous research and baseline research

Table 6 presents a detailed comparison between the results of the current study, previous works, and a baseline reference. This comparison emphasizes the performance improvements achieved, showcasing the effectiveness and advantages of the proposed method.

Table 6. Comparison of efficiency and key parameters across different years.

Year	Eff. (%)	FF (%)	Voc (V)	Isc (mA/cm ²)	Reference
2016	22.61	80.6	0.741	37.8	[20]
2019	23.35	80.4	0.734	39.5	[21]
2023	23.64	80.5	0.767	38.3	[22]
Baseline Research	24.34	85.02	0.98	29.10	[12]
Present Study	32.85	83.2	0.63	62.41	-

Moreover, optimizing the thickness of the upper layers, including CdS and TCO, reduced optical losses and improved light transmission to the absorber layer, thereby contributing to the overall efficiency enhancement [23-24].

Increase in fill factor (FF = 83.2%)

This study reports a Fill Factor (FF) higher than previously published values, although slightly below the baseline research value of 85.02%. The FF improvement is mainly attributed to a reduction in series resistance (Rs) achieved by optimizing internal electrical connections and enhancing contact quality, which

minimized resistive losses and directly increased FF [25-26]. Additionally, improvements in the layer growth process and deposition techniques reduced electronic defects and energy losses, further enhancing the FF. The incorporation of advanced transparent materials in the upper layers also contributed by promoting electric field uniformity, reducing charge carrier recombination, and thereby boosting the FF [27].

Increase in short-circuit current ($ISC = 62.41 \text{ mA/cm}^2$)

The recorded short-circuit current density (J_{sc}) of 62.41 mA/cm^2 represents a substantial improvement compared to previous studies, where the highest reported J_{sc} was 26.3 mA/cm^2 in 2015 [28], and the baseline study reported 29.10 mA/cm^2 [12]. This enhancement is attributed to several key factors: optimized absorber layer composition and thickness adjustment, which broadened and improved light absorption across the spectrum [29]; improved crystal quality through the reduction of structural defects in the CIGS layer, increasing charge carrier collection efficiency; and minimized optical losses by enhancing the transparency and optimizing the thickness of upper layers, thereby reducing photon losses and enabling a higher J_{sc} [30].

Open-circuit voltage ($VOC = 0.63 \text{ V}$)

The achieved open-circuit voltage (V_{oc}) of 0.63 V is lower than values reported in previous studies— 0.98 V in the baseline and higher values in 2015 and 2019—but remains a critical parameter for further optimization. V_{oc} is influenced by several factors, including internal quantum efficiency; notably, an increase in short-circuit current density (J_{sc}) often accompanies a slight decrease in V_{oc} due to bandgap tuning. Additionally, carrier recombination caused by a weaker internal electric field leads to charge carriers recombining before collection, reducing V_{oc} . Nevertheless, there is substantial potential for improvement through optimizing interface layers and incorporating novel materials to minimize V_{oc} losses and further boost CIGS solar cell performance [31-32].

Conclusion

This study demonstrates a record-breaking efficiency of 32.85%, significantly exceeding previous benchmarks. These improvements result from optimized absorber layer composition, reduced recombination losses, enhanced material properties, and refined device architecture. Although further refinement of the open-circuit voltage (V_{oc}) is needed, the overall results provide a solid foundation for future advancements in CIGS solar cell technology. The maximum power output was determined using Invasive Weed Optimization (IWO), a powerful algorithm employed to maximize system performance.

Conflict of Interest

The authors declare that there are no potential conflicts of interest associated with the publication of this work.

Abbreviations

IWO	Invasive Weed Optimization
FF	Fill Factor
V_{oc}	Open-Circuit Voltage
I_{sc}	Short-Circuit Current
J_{sc}	Short-Circuit Current Density
TCO	Transparent Conductive Oxide
ZnO	Zinc Oxide
CdS	Cadmium Sulfide
Mo	Molybdenum
Pm	Maximum Power Output
V_m	Voltage at maximum power
I_m	Current at maximum power
Eff	Energy Conversion Efficiency

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