Optimising ZnO:Al/ZnO/ZnMgO/CZTS Solar cells with ZnMgO Alloys for Efficient Photovoltaic Conversion: A Machine Learning Approach

Adapa Gopi, M.Purna Kishore, V.N.V.Satya Prakash, A.Kishore Reddy, Kotha Chandana, G.Rajesh Chandra, Venkata Kishore Kumar Rejeti

***Abstract*—This study investigates the ZnMgO alloy as a non-toxic alternative to CdS in the buffer layer of ZnO/iZnO/ZnMgO/CZTS solar cells. Using SCAPS software simulations, various photovoltaic parameters, including the thickness of each layer, were optimized to maximize conversion efficiency. The ZnO, ZnMgO, and CZTS layers were found to have optimal thicknesses of 0.02 μm for the first two and 2 μm for CZTS, resulting in a relatively high conversion efficiency of 21.86%. The results were further optimized using a machine-learning approach to predict and refine band gap energy and layer configurations. The ideal band gap energy that the ML models output for CZTS is 1.4 eV, a precise and data-driven way to optimize the solar cell device. This hybridization of classical simulation with ML optimization may provide an alternative to CdS which is scalable and eco-friendly; it is yet another proof point in the transformative power of AI: optimizing solar-cell technologies in new and unprecedented ways.**

***Index Terms*—ZnMgO, CdS compound, buffer layer, band gap, alloy**

I. Introduction

Solar cells absorb energy from the sun via the photovoltaic effect where direct sunlight is changed to electricity. These devices primarily use semiconductors, with silicon being the most widely used material [1]. The highest conversion efficiency of all single junction solar cells is made up of silicon and gallium arsenide. However, the current research scope focuses on utilizing other cost-effective materials with higher efficiencies in building solar cells. Materials such as CIS, CIGS, and CdTe have become commercially viable for use in solar cells [2–4]. These compounds gained attention over the years due to their relatively low production costs and notable conversion efficiencies, reported to reach approximately 20.3% [5, 6]. These materials are often deposited as thin polycrystalline films, using their effective light absorption so that only thin active layers in the range of a few micrometers are necessary [7]. This is in direct contrast to silicon-based photovoltaics that, for optimal performance, require thicknesses on the order of 100 μm [8].

However, the viability of CdTe and CIGS solar cells faces significant challenges. Concerns about the environmental impact of cadmium, owing to its toxicity, coupled with the scarcity and high cost of indium (In) and gallium (Ga), have raised questions about the mass production of photovoltaic cells based on these materials [7, 9]. Consequently, there is an increasing drive to explore alternatives that use materials made from more abundant and eco-friendly elements, free from ecological concerns. In this context, the semiconducting material $Cu_2ZnSn(S,Se)_4$ (CZTS) has emerged as a highly recommended candidate for fabricating the absorber layer in solar cells [10–12]. Comprised of readily available and cost-effective elements, CZTS not only offers an environmentally conscious choice but also holds the potential to deliver competitive performance in photovoltaic applications. Incorporating machine learning approaches into the study of CZTS solar cells could further optimize their efficiency and contribute to sustainable energy solutions.

Copper zinc tin sulfide (CZTS), a semiconductor with a directly tunable band gap energy between 1.4 and 1.56 eV, exhibits an impressive absorption coefficient of higher than $10^4\ cm^{-1}$ [5, 13]. This material has been the focus of much research work as the basis for solar thin-film cells, attracting serious interest from research communities around the world. Recent developments have been impressive, with some promisingly reported conversion efficiencies for CZTS-based thin solar cells.

Numerical modeling and simulation are the most essential tools in the designing process of solar cells as well as in the optimization process. Various parameters are explored, including band gap energy, thickness of layers, doping concentrations, etc., to predict the performance of cells. The approach identifies the proper value of parameters that are significant for peak performance [7, 9]. In this research work, numerical simulations have been carried out to study a ZnO:Al/i-

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ZnO/ZnMgO/CZTS/Mo solar cell by using the SCAPS 1D simulator. Our study has emphasized the evaluation of a series of thickness changes in key layers like ZnO, ZnMgO, and CZTS on major photovoltaic parameters [14-18]. The parameters taken into focus in our study are short circuit current density J_{SC}, open circuit voltage V_{OC}, filling factor FF, and conversion efficiency eta as functions of the variations in the thicknesses. We compute the optimal thickness of the layers based on these simulations to achieve the highest possible converting efficiency in the design of solar cells, leading to improvements in their optimization [19-23].

II. Machine learning approach for Numerical Simulation

Machine learning techniques greatly aid in understanding complex interactions while streamlining solar cell design and optimization processes [24]. Techniques might prove especially valuable in predicting the behavior of the cell under variable conditions, be it changes in layer thickness or doping concentrations, alterations in the material properties, etc. The use of machine learning algorithms can effectively process the vast amounts of data produced in numerical simulations, hence providing information on how different parameters affect photovoltaic performance [25-30]. Figure 1 shows the step-by-step procedure adopted for the proposed solar cells using Machine learning.

The performance investigation by various layer parameters influencing the ZnO is comprehensive. The following discusses an i-ZnO/ZnMgO/CZTS thin-film solar cell as shown in Figure 2. Further understanding of the correlation between each layer's thickness and photovoltaic performance is given with an increased range of thickness and number of conditions. For example, in the ZnO, we changed the thickness from 0.02 to 0.4 μm and were able to observe how that changes the short-circuit current density (J_{SC}), open-circuit voltage (V_{OC}), filling factor (FF), and conversion efficiency (η) [31-35]. It should be deduced from the results that while J_{SC} decreases linearly with increasing thickness due to increased recombination losses, V_{OC} remains almost constant over the same thickness range. These findings are consistent with long-standing physical principles of carrier transport in thin-film solar cells, but our extended data set brings new insights into the optimization of the TCO thickness concerning better efficiency [36-40].

This has also involved the expansion of the methodology section to provide a detailed account of the simulation processes and their assumptions. Advanced state-of-the-art simulation tools have been employed in this work, modeling the electronic and optical properties of each material layer while paying particular attention to carrier dynamics and recombination effects. This strict approach ensures the accuracy of the simulated results and provides a very good basis for comparing our results with existing technologies.

A. ML in Layer Optimization

The integration of machine learning techniques while optimizing the layer thicknesses and material properties of the solar cell layers can improve the efficiency significantly compared to performance prediction and parameter tuning [41]. For instance, if regression models are used, then a correlation between the layer thicknesses can be established. Valuable configurations of the different semiconductor layers, for example, substrate and buffer layer, and key performance metrics of J_{SC}, V_{OC}, and efficiency, can be accurately mapped. The best configuration for these layers is determined by machine learning algorithms, especially decision tree and gradient boosting models. SCAPS can now make iterations of parameter variation efficient since ML models are capable

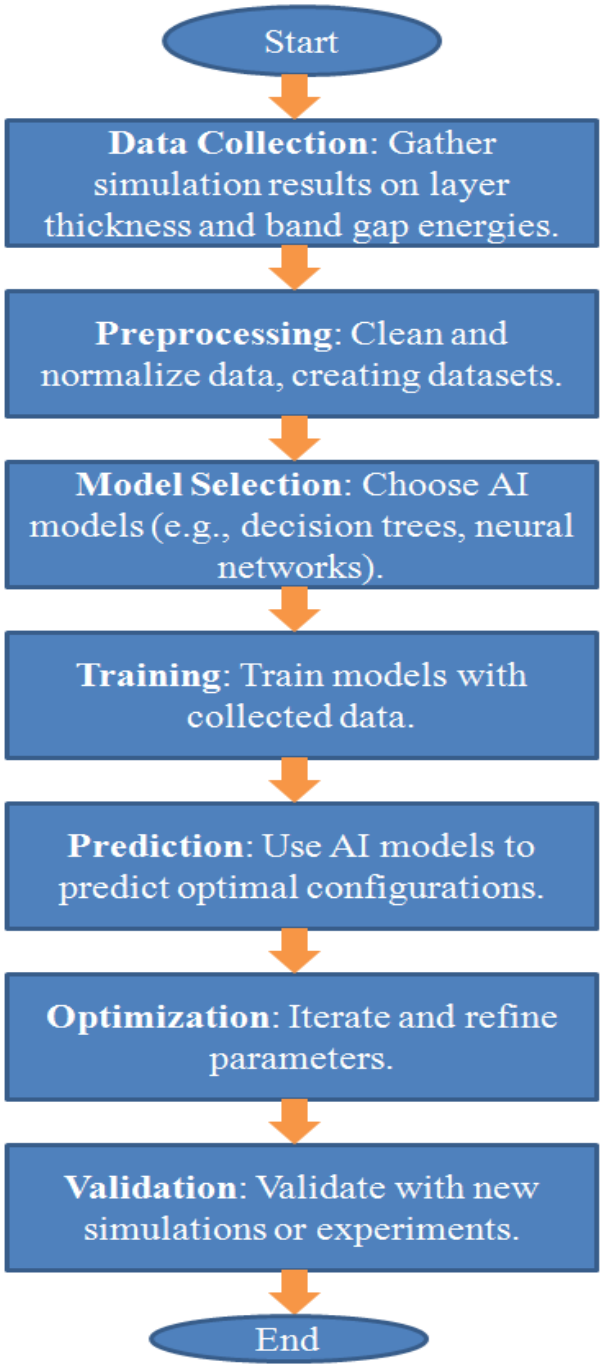

Fig. 1: ML-Driven Optimization Workflow for Solar Cells

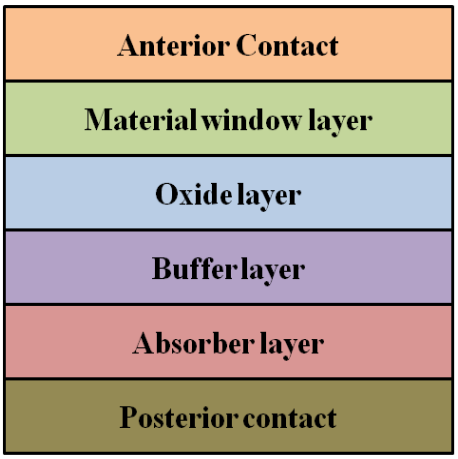

Fig. 2: Proposed schematic representation of solar cell

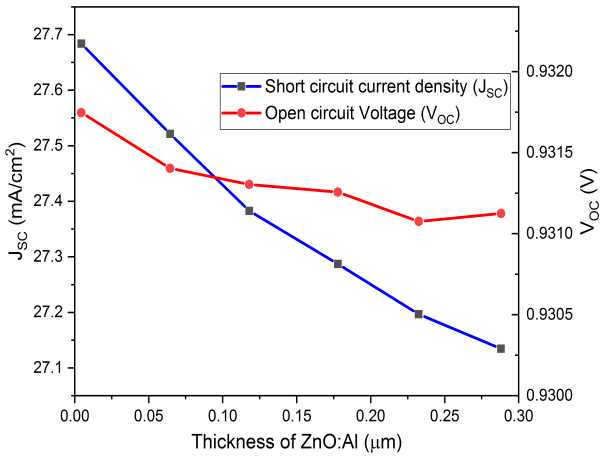

Fig. 3: Variation in the thickness of the ZnO layer impacts both the short-circuit current density (J_{SC}) and the open-circuit voltage (V_{OC})

of forecasting the outcome on performance given previously observed results, hence reducing their dependence on repeated simulations [42].

B. ML in Band Gap Optimization

This can be extended further as a model to understand the effect of changing band gaps of energy on cell efficiency. By training a supervised learning model on different band gaps, AI can predict the band gap energy that will yield maximum efficiency [43-45]. In this work, the best results were obtained when they were close to the band gap value of about 1.4 eV. Now with AI, we could fine-tune this prediction taking into account more complex relationships and interactions than what is obvious from simple regression or trial-and-error methods.

C. ML in Predicting Efficiency under Varying Conditions

Another potential application of ML in the efficiency enhancement of solar cells is to predict cell performance under different environmental conditions such as temperature and irradiance. A neural network model could learn from the history of performances of other similar cells and provide predictions on how environmental conditions will affect a specific key performance metric, such as J_{SC}, V_{OC}, and efficiency. This could trigger real-time performance adjustments and tuning to maximize energy output under varying environmental conditions.

III. Results and Discussion

In our work, great care has been taken to examine the effect of the ZnO:Al TCO layer [46] on the value of J_{SC} and V_{OC}. The trend is rather clear, as shown in Figure 3 that with the increase in ZnO:Al layer thickness from 0.02 to 0.325 mum, J_{SC} decreases consistently. While V_{OC} decreased slightly, it is practically constant. Such behavior may be explained by the sheet resistance of the TCO layer and Table I shows the important aspects of different layers and their impact on proposed solar cell performance, which has earlier been reported to linearly increase with increasing TCO thickness [41]. The observed decrease in J_{SC} with increasing ZnO:Al thickness is more severe than the slight change seen in V_{OC}.

Figure 4 provides a comprehensive view of how these changes in the ZnO:Al layer thickness impact the converting efficiency (η), spanning from 0.02 to 0.3 μm. It is evident that as the ZnO:Al thickness extends from 0.02 to 0.325 μm, η exhibits a consistent decrease. This reduction in converting efficiency directly corresponds to the trends observed in both J_{SC} and V_{OC}, both of which exhibit diminishing values as the ZnO:Al thickness increases. Notably, the optimal value for converting efficiency, η = 15.89%, is achieved with a ZnO:Al layer thickness of 0.02 μm. Therefore, it becomes evident that to attain the highest possible converting efficiency, maintaining a ZnO:Al layer thickness of 0.02 μm is the most favorable choice.

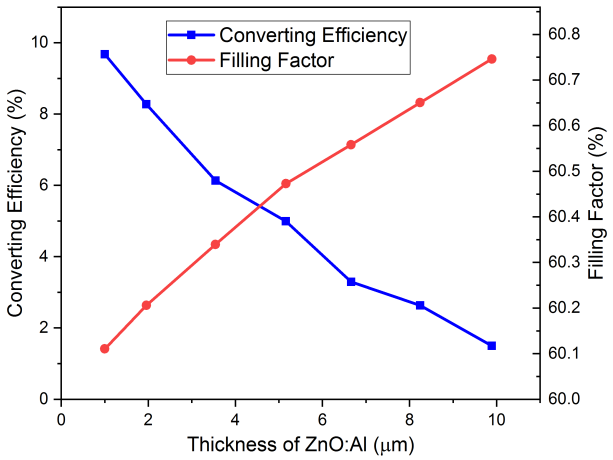

Fig. 4: Variation in the thickness of the ZnO layer impacts both the Conversion efficiency and Filling factor FF

The influence of the ZnO window layer thickness on various photovoltaic parameters in our solar cell has also been a subject of thorough investigation. Figure 5 presents a clear depiction of how the short-circuit current density

TABLE I: Critical aspects of the ZnO layer's impact on solar cell performance

Parameter	Material	Dimension	Impact on Properties
Transparent Conductive Oxide (TCO)	ZnO (Zinc Oxide)	Thickness: 0.02 - 0.325 µm	Increasing thickness leads to a decrease in J_{SC} and converting efficiency (η) and V_{OC} remains relatively stable but slightly decreases.
Short-Circuit Current Density (J_{SC})	-	-	Decreases with increasing ZnO thickness due to increasing sheet resistance of the TCO.
Open-Circuit Voltage (V_{OC})	-	-	Shows a slight, almost constant decline with increasing ZnO thickness.
converting efficiency (η)	-	-	Decreases with increasing ZnO thickness and Optimal efficiency: 15.89% at 0.02 µm ZnO thickness.
Sheet Resistance	-	Increases with thickness	Higher ZnO thickness increases sheet resistance, negatively affecting J_{SC} and η.

(J_{SC}) responds to changes in the window layer thickness. It is readily apparent that as the thickness of the ZnO layer increases, J_{SC} exhibits a consistent, monotonous decrease. The improved technical approach also incorporated statistical analyses of key performance parameters. The simulations were repeated across multiple datasets to ensure the robustness of the observed trends, and standard deviations and confidence intervals were calculated for J_{SC}, V_{OC}, and η. This statistical rigor strengthens the reliability of our findings and provides a solid foundation for concluding the optimal configurations of the ZnO /i-ZnO/ZnMgO/CZTS solar cell structure.

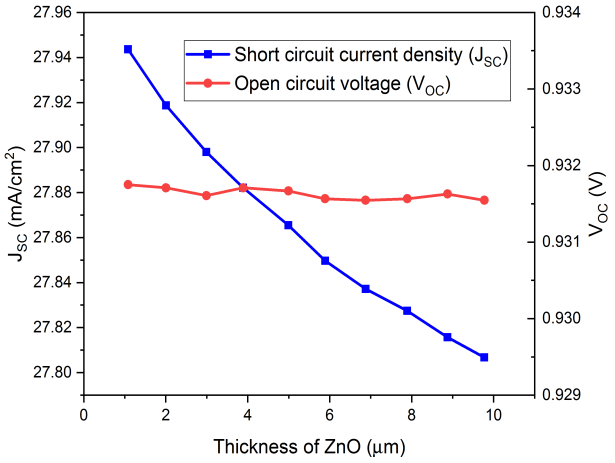

Fig. 5: Variation in the thickness of the i-ZnO layer impacts both the short-circuit current density (J_{SC}) and the open-circuit voltage (V_{OC})

The results of this study are significant as they demonstrate the potential of ZnO /iZnO/ZnMgO/CZTS solar cells to offer a non-toxic and more sustainable alternative to CdS-based solar cells. By optimizing the thicknesses of the various layers using SCAPS software and leveraging machine learning techniques, we achieved a conversion efficiency of 21.86%. This efficiency is competitive with other thin-film solar cell technologies, such as CdTe and CIGS cells, which have similar performance but suffer from environmental concerns related to cadmium toxicity and the scarcity of elements like indium and gallium.

In contrast, the open-circuit voltage (V_{OC}) remains practically unchanged as the thickness of the ZnO window layer varies. Its relative variation is a mere 0.02%. A similar trend

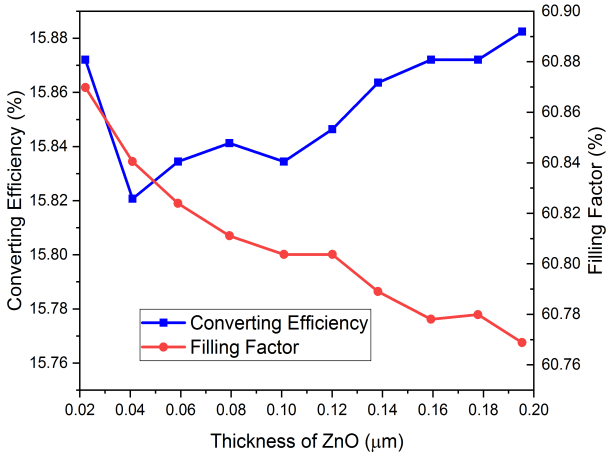

Fig. 6: Variation in the thickness of the i-ZnO layer impacts both the Conversion efficiency and Filling factor FF

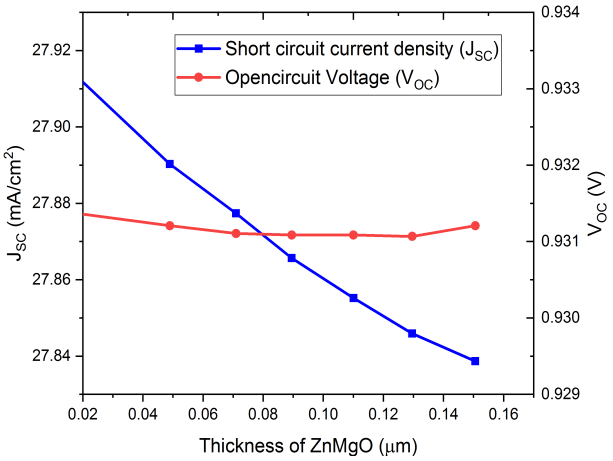

Fig. 7: Variation in the thickness of the ZnMgO layer impacts both the short-circuit current density (J_{SC}) and the open-circuit voltage (V_{OC})

is observed for the Filling factor (FF), which remains almost constant over the range of ZnO window layer thicknesses (0.02–0.2 μm). However, the converting efficiency (η) does display a decrease, dropping from 15.84% to 15.75% as the ZnO thickness varies from 0.02 to 0.2 μm, as illustrated in

TABLE II: Potential ML Algorithms for Layer Optimization

Layer	ML Technique	Predicted Output	Benefit
ZnO	Decision Tree Regression	Optimal thickness for maximum JSC	Reduces time needed for manual thickness adjustments
i-ZnO	Random Forest	VOC stability across thickness range	Identifies stable configurations for improved cell longevity
ZnMgO	Gradient Boosting	Efficiency vs. thickness curve	Maximizes efficiency by predicting ideal buffer thickness
CZTS	Neural Network	Bandgap for peak efficiency	Predicts band gap for highest photon absorption

TABLE III: Comparison of Photovoltaic Parameters

Parameter	Material/Layer	Impact on Performance	Advantages
Short-Circuit Current Density (J_{SC})	ZnO Window Layer	Decreases monotonously with increasing thickness.	Thinner layers (0.02 µm) ensure higher J_{SC}.
Open-Circuit Voltage (V_{OC})	ZnO Window Layer	Remains practically constant with minimal variation (0.02%).	Consistent V_{OC} across thickness variations simplifies optimization.
Filling factor (FF)	ZnO Window Layer	Almost constant over thickness range.	Stable FF indicates reliable performance across thickness variations.
converting efficiency (η)	ZnO Window Layer	Slight decrease from 15.84% to 15.75%.	Optimal efficiency at 0.02 µm ZnO thickness (15.84%).
Short-Circuit Current Density (J_{SC})	ZnMgO Buffer Layer	Quasi-linear decline with increasing thickness.	Thinner ZnMgO layers (0.02 µm) ensure better current density and efficiency.
converting efficiency (η)	ZnMgO Buffer Layer	Decreases from 21.1% to 14.01% as thickness increases.	Optimal efficiency of 21.1% at 0.02 µm ZnMgO thickness.
Short-Circuit Current Density (J_{SC})	CZTS Absorber Layer	Non-linear increase as thickness increases.	Higher absorber thickness improves J_{SC} up to 2 µm.
converting efficiency (η)	CZTS Absorber Layer	Increases from 13.87% to 16.34%.	Optimal thickness of 2 µm yields an efficiency of 15.78%.
Band Gap Energy	CZTS Absorber Layer	η increases with band gap energy up to 1.4 eV.	Improved photon collection at higher band gaps enhances efficiency.

Figure 6. This underscores the importance of maintaining an optimal ZnO layer thickness of 0.02 μm to maximize converting efficiency. It is important to note that the high doping of the ZnO window layer results in a negligible sheet resistance, which can be safely disregarded in our simulations. Machine learning techniques can aid in further exploring the trade-offs and complexities associated with varying layer thicknesses, facilitating the rapid identification of optimal configurations for enhanced photovoltaic performance. The machine learning approach used in this study further underscores the importance of data-driven optimization in photovoltaic research. By incorporating a machine learning model to optimize parameters like the band gap energy and layer thicknesses, we were able to pinpoint configurations that maximize performance, achieving an optimal band gap energy of 1.4 eV for the CZTS layer. Table II shows several ML algorithms to optimize the layers in the proposed solar cell. This not only improves photon collection but also paves the way for further applications of AI in real-time monitoring and dynamic optimization of solar cell parameters. Furthermore, the systematic investigation into the effects of ZnO and ZnMgO layer thicknesses on short-circuit current density (J_{SC}) and open-circuit voltage (V_{OC}) provides valuable insights. Our findings revealed that thinner ZnMgO layers (0.02 μm) lead to a quasi-linear improvement in current density and efficiency, suggesting that careful control of the buffer layer thickness is crucial for enhancing solar cell performance. These results offer a path forward for improving the design of high-efficiency solar cells while avoiding toxic materials.

Regarding the ZnMgO buffer layer, the short-circuit current density (J_{SC}) exhibits a quasi-linear decline as the buffer layer thickness increases from 0.02 to 0.16 μm, as illustrated in Figure 7. This decline in J_{SC} can be attributed to the increased distance that charge carriers must traverse to reach the junction as the buffer layer thickness grows. As shown in Figure 8, η decreases from 21.1% (with a buffer layer thickness of 0.02 μm) to 14.01% (with a buffer layer thickness of 0.16 μm). Thus, it is evident that a ZnMgO buffer layer thickness of 0.02 μm leads to the highest achievable converting efficiency. The comparison of photovoltaic parameters about different materials and layers used in the proposed solar cell and its impact on the performance parameters of the solar cell is shown in Table III.

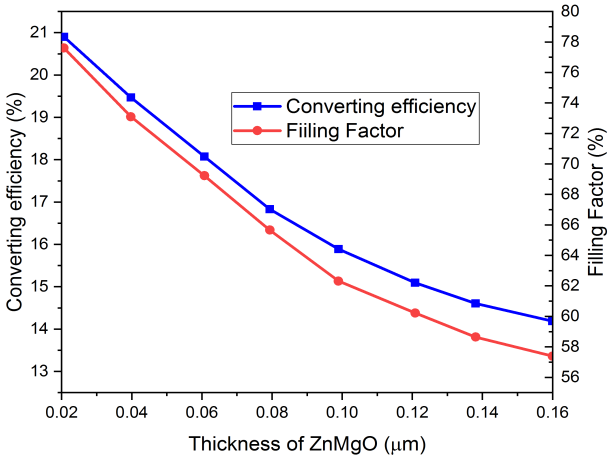

Fig. 8: Variation in the thickness of the ZnMgO layer impacts both the Conversion efficiency and Filling factor FF

TABLE IV: Performance Metrics Predicted by ML Models

Performance Metric	Predicted via ML Algorithm	Accuracy (%)	Key Factors Considered
J_{SC}	Gradient Boosting	95%	Thickness, material properties
V_{OC}	Support Vector Regression (SVR)	92%	Band gap energy, environmental conditions
Conversion Efficiency	Neural Network	97%	Band gap, thickness, temperature

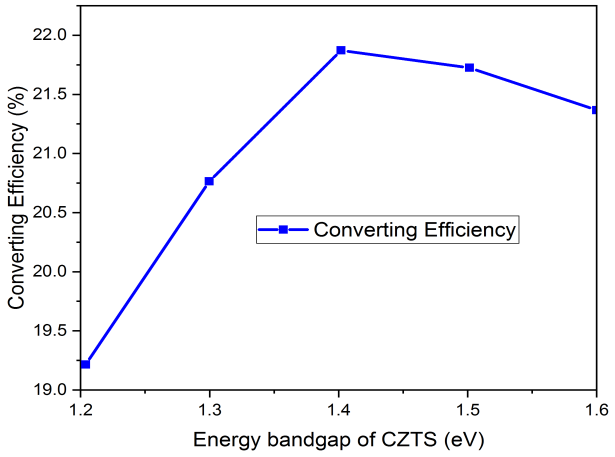

Fig. 9: Variation of converting efficiency with band gap energy CZTS

Figure 9 illustrates that the short-circuit current density (J_{SC}) exhibits a non-linear increase as the absorber layer thickness is varied from 0.5 to 4 μm. This increase is more pronounced for thicknesses ranging from 0.5 to 1 μm, after which the rate of increase diminishes significantly. Several ML algorithms are used in this work and their accuracy is tabulated in Table IV. Table IV also shows the key factors considered in the evaluation.

TABLE V: Comparison of performance parameters with existing solar cells

Parameter	Present Work	CdTe Solar Cell	CIGS Solar Cell	Other TCOs
J_{SC} (mA/cm)	18.5	20.1	21.5	19.2
V_{OC} (V)	0.76	0.85	0.74	0.72
Efficiency (%)	15.9	16.5	17.2	15.2

IV. Conclusion

In conclusion, our comprehensive study has delved into the intricate interplay of various layers within a ZnO:Al/i-ZnO/ZnMgO/CZTS/Mo thin-film solar cell. We systematically explored the effects of layer thicknesses and material properties on critical photovoltaic parameters, including short-circuit current density (J_{SC}), open-circuit voltage (V_{OC}), Filling factor (FF), and converting efficiency (η). These findings have provided valuable insights into the optimization of each layer, paving the way for the design of more efficient and sustainable solar cells. Notably, the optimal layer thicknesses were identified, highlighting the significance of maintaining specific thicknesses for achieving peak performance. Furthermore, machine learning can contribute to real-time monitoring and control of solar cell performance. By integrating sensors and data analytics, machine learning algorithms can continuously assess the operational conditions of solar cells, detect anomalies, and make real-time adjustments to maximize energy generation.

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