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Research Article

Low-Cost ZnO/Perovskite Solar Cells, Fabrication, Simulation, and Performance Optimization

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Abstract **–** This study describes an in depth study into fabrication and simulation of low cost ZnO/ perovskite (PSC) solar cells using SCAPS-1D. The interest is in making material selection, structural parameters, and deposition techniques to improve photovoltaic performance without raising the price. Employing ZnO as the electron transport layer was driven by the high electron mobility, optical transparency, and ability to use low temperature methods such as spin-coating. This approach is applied for the deposition of ZnO seed layer that encourages uniform nanorod growth, followed by the solution based deposition of methylammonium lead iodide ($MAPbI_3$) perovskite films. ITO, NiO, $CH_3NH_3PbI_3$, ZnO layers were used to construct a ZnO-based perovskite solar cells device structure. The influence of active layer thickness and acceptor density was analysed in a systematic manner. Results indicated NiOlayer thicknesses ranged between 2–3 μm and optimal doping levels producing optimum performance with JSC of ~18.70 mA/cm² and efficiency up to 17.15%. Conversely, excessive thickness increased resistance and recombination. The perovskite layer demonstrated high sensitivity to doping, with PCE dropping from24.35% to 22.47% as acceptor density decreased. In contrast, ZnO layer modifications had minimal impact, showing efficiency stability around 17.19–17.20%. Thermal effects were also evaluated; as temperature rose from 300 K to 350 K, Voc declined from 1.10 V to 1.02 V and efficiency dropped to 15.3%, confirming the importance of thermal stability. External quantum efficiency (EQE) peaked at 90%near 400 nm, affirming strong visible light absorption. Overall, this work highlights ZnO-perovskite hybrid structures as a promising, scalable, and eco-friendly alternative for next- generation photovoltaics, offering a balance between cost, process simplicity, and performance.

Keywords – PSC, ZnO, Low-Cost Fabrication, SCAPS-1D Simulation, Thermal Stability.

I. INTRODUCTION

Recent advancements in solar cell technology have been driven by the growing demand for sustainable and renewable energy sources, particularly in the development of low-cost and efficient photovoltaic materials. While conventional solar cells primarily utilize silicon as the semiconductor material, the high cost of silicon remains a major challenge for widespread adoption. As a result, developing cost-effective alternatives has become critical. Among these oxide semiconductors, e.g., ZnO have become interesting

candidates. The combination of two different structures such as zinc oxide(ZnO) and perovskite structures have become an attractive strategy for improving solar energy conversion efficiency with the reduced cost of production. ZnO withits desirable electronic properties and availability, is a good electron transport layer insolar cells while perovskite-type materials are highly appreciated for the high absorption coefficient and tunable bandgaps [1],[2],[3].

Solar cells also known as photovoltaic (PV) devices work by converting Sunlight is transformed into electricity by means of the photovoltaic effect. Silicon (Si) has traditionally had a firm status as the material of choice as a main semiconductor element in solar cells because of its high level of efficiency (22–27% for products destined for commercial use) and stability in long-term operation. However, recent innovations have provided perovskit materials as potential – heavy contenders in the next generation of solar technology [4],[5].

Perovskites feature a distinctive cubic crystal lattice arrangement of cations and anions, enabling them to exhibit remarkable properties such as rapid charge generation, high carrier mobility, an optimal bandgap for solar absorption, low exciton binding energies, and suppressed recombination rates compared to conventional materials. Perovskite solar cells (PSCs) exhibit exceptional properties that make them a leading candidate for next-generation photovoltaics. Their advantages include high efficiency, improved material stability, cost-effective production, and simple processing methods. A key component of PSCs is the electron transport layer, which is essential for efficiently collecting and transferring electrons from the photoactive layer to the electrode. Achieving an optimal thickness for the compact electron layer is essential, as it not only enhances electron collection efficiency but also helps minimize the formation of pinholes, which can otherwise compromise device performance [6],[7].

Zinc oxide is extensively utilized in solar cell fabrication because of high optical transparencies, low cost and rapid electron mobility as well as adjustable conductivity. As a carrier transport layer in PSCs, ZnO increases carrier transport efficiency, and reduces recombination losses which has enhanced device performance. The production of ZnO layers of relatively low cost frequently uses straightforward solution-processable methods such as sol-gel, water bath and combustion synthetic procedures causing the formation of various ZnO nanoforms such as nano-wires and nano-particles. These nanostructures may build mesoporous layers thus increasing the contact area to perovskite films, which enhances charge extraction and higher solar cells efficiency. Moreover, low-temperature processing and environmentally-friendly properties of ZnO quite prospective material for sustainable and inexpensive solar energy. Also, such materials as TiO_2, ZnO and SnO_2 are widely used as the electron transport layers. Each of the materials possesses specific benefits, ZnO being superior in regards to cheap fabrication, ease of processing at low temperatures and availability of flexible substrates [8],[9],[10]. Material optimization is still of utmost importance for the progress of the perovskite solar cell (PSC) technology as shown by complementary studies of the experimental and computational approaches. Although Aseena et al. (2019) argued the beneficial performance of ZnO/Cu_2O charge transport layers, further investigation by Uddin et al. (2025) identified the same dual advantages of ZnO in efficiency and environmental safety, when the latter is used with $MAPbI_3/MASnI_3$ absorbers. These results are further supported by the seminal SCAPS-1D simulations of Park et al. (2024) that were able to achieve 23.84% efficiency in $ZnO/CsSnI_3$ configurations by optimizing the thickness and doping precisely enough – highlighting how targeted material engineering can concurrently improve efficiency, minimize the presence of lead, and slew the commercialization pathway of sustainable photovoltaics: [11][12].

Moreover, researchers have explored alternative charge transport materials in perovskite solar cells has yielded significant insights into both organic and inorganic alternatives. While polymeric HTLs like P3HT improve device longevity [13], inorganic options (CuI [14], PbS [15], CuSCN [16] for HTLs; TiO_2 [17],[18], ZnO [19] for ETLs) offer enhanced stability and cost-effectiveness [13,14]. Particularly for electron transport layers, Kaya et al. (2024) demonstrated that TiO_2 synthesis methodology critically impacts performance - their acetylacetone-assisted approach produced crack-free films that enabled mesoporous devices (0.1% PCE) to outperform planar architectures (0.03% PCE), underscoring how material quality and processing techniques collectively determine PSC efficiency [20].

This study explores the simulation of low-cost ZnO/perovskite solar cells usingSCAPS-1D, alongside fabrication techniques aimed at advancing economically viable solar energy solutions. By harnessing the potential of ZnO/perovskite hybrid systems.

II. MATERIALS AND METHOD

Perovskite solar cells have been receiving increasing interest in the past few years owing to this material's power conversion efficiencies, ability to tune bandgaps as well as its ease of fabrication. Out of all other architectures proposed, the ZnO-based perovskite solar cell structures that can be made with less expensive inputs have proven to be very promising in terms of large scale deployment. In this work zinc oxide (ZnO) was chosen as the ETL due to its high electron mobility, its ambient stability and because it is suitable for the solution processing, which is consistent with the aim of low-cost cost-effective fabrication.

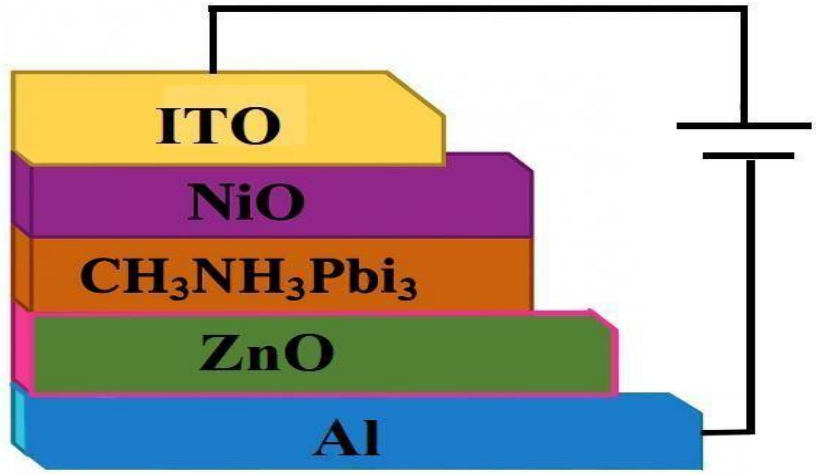

Figure 1 Schematic of the fabricated ZnO-based perovskite solar cell

Figure 1 illustrates the schematic structure of the fabricated low-cost ZnO/perovskite solar cell, where each functional layer plays a critical role in determining the device's photovoltaic performance. The structure begins with a transparent bottom electrode made of indium tin oxide (ITO), which serves as the hole-collecting contact. Above this, a p-type nickel oxide (NiO) layer functions as the hole transport layer (HTL). Next, the methylammonium lead iodide ($CH_3NH_3PbI_3$) perovskite absorber layer absorbs sunlight and generates charge carriers. An n-type zinc oxide (ZnO) electron transport layer (ETL) facilitates electron extraction, while a thermally evaporated aluminum (Al) back electrode completes the electrical circuit.

In order to check the performance of the fabricated ZnO-based perovskite solar cell illustrated in Figure 1, one-dimensional numerical simulations have been performed employing SCAPS-1D. The Layered Semiconductor Device Model (LCDM) simulation software solves Poisson's equation and the continuity equations for electrons and holes to simulate layered semiconductor devices. The simulation parameters including the layer thicknesses, bandgap, carrier mobilities, the parameters and defect densities for each layer are listed in Table 1.

Table 1 Input parameters for SCAPS-1D simulation of ZnO-based perovskite solar cells

Parameter	ITO	NiO	$CH_3NH_3PbI_3$	ZnO (ETL)
Thickness (nm)	40	40	200	40
Bandgap (eV)	3.500	3.500	1.500	3.300
Electron Affinity (eV)	4.000	2.200	3.900	4.000
Dielectric Permittivity	9.000	9.000	10.000	9.000
Nc ($1/cm^3$)	2.200E+18	3.000E+19	8.000E+20	4.000E+18
Nv ($1/cm^3$)	1.800E+19	2.000E+19	8.000E+19	2.000E+19
v_e,th(cm/s)	1.000E+7	1.000E+7	1.000E+7	1.000E+7
v_h,th(cm/s)	1.000E+7	1.000E+7	1.000E+7	1.000E+7
μ_e (cm^2/Vs)	3.000E+1	1.200E+1	1.00E+1	1.000E+2
μ_h (cm^2/Vs)	5.000E+0	5.000E+0	1.000E+1	3.000E+1
ND ($1/cm^3$)	2.000E+20	0.000E+0	1.000E+15	1.000E+19
NA ($1/cm^3$)	0.000E+0	2.000E+19	2.000E+0	0.000E+0

The layered architecture employs low-temperature, solution-processed methods, making it compatible with flexible substrates and scalable manufacturing. By optimizing material selection and deposition processes, this design balances performance with affordability, a critical requirement for next-generation photovoltaics. The fabrication involves sequential deposition of functional layers under ambient or mild thermal conditions, as detailed below.

A. Substrate Cleaning and Preparation for Low-Cost ZnO-Based PerovskiteSolar Cells

A clean substrate is vital for efficient ZnO-based perovskite solar cells. ITO-coated glass is etched using an HCl\:H_2SO_4\:H_2O solution to define the active area. Ultrasonic cleaning is performed on the substrates with detergent, deionized water, acetone, and isopropanol before drying them with nitrogen gas. Optional UV-ozone treatment enhances surface wettability. This low-cost process ensures good film adhesion and electrical contact, critical for high-performance device fabrication[20][21].

B. Deposition of the ZnO layer

The ZnO seed layer is deposited to promote uniform nanorod growth using a low-cost, ambient-temperature spin coating method instead of traditional high-temperature techniques. A precursor solution, made from zinc acetate or nitrate in ethanol or 2-propanol with stabilizers like ethanolamine, is spin-coated onto a cleaned FTO substrate at ~3000 rpm for 30 seconds. Multiple coatings improve film uniformity. Afterward, the substrate is dried at ~30°C for 10 minutes. Aging the coated substrate under ambient conditions for at least 24 hours enhances crystallinity and adhesion for effective ZnO nanostructure formation[22],[23].

C. Deposition of the $CH_3NH_3PbI_3$ Layer

The perovskite layer is formed by spin-coating a PbI_2 solution onto a ZnO nanorod array, followed by low-temperature annealing (~70 °C). Methylammonium iodide (CH_3NH_3I) is then deposited via two-step spin-coating and annealed at ~80 °C. This straightforward, all-solution process enables perovskite crystallization and uniform film formation under ambient conditions, eliminating the need for inert atmospheres and reducing fabrication costs [22].

D. NiO Layer (HTL) Fabrication

Nickel oxide is widely used as a low-cost and robust hole transport layer (HTL) in inverted perovskite solar cells, working alongside ZnO for efficient charge extraction. Its p-type conductivity, wide bandgap, and chemical stability enable efficient hole extraction and electron blocking. NiOx can be deposited using low-temperature methods like spin coating. Doping with metal cations and adding interface modifiers further enhance conductivity, stability, and device performance [24].

III. RESULTS AND DISCUSSION

The investigation into low-cost ZnO/perovskite solar cells demonstrates promising enhancements in photovoltaic performance through material optimization, particularly concerning the thickness of hole and electron transport layers, temperature effects, and doping strategies.

The J–V characteristics under illumination Figure 2 reveal typical diode behavior with a high open-circuit voltage (Voc) of approximately 1.1062 V and a short-circuit current density (Jsc) near −20 mA/cm², fill factor (FF) of 83.21%, and an efficiency (η) of 17.15%, indicating efficient charge separation and collection. The steep rise of the curve and the marked data points underscore consistent device performance, aligning with previous studies that associate sharp J–V profiles with low recombination losses and high-quality device fabrication.

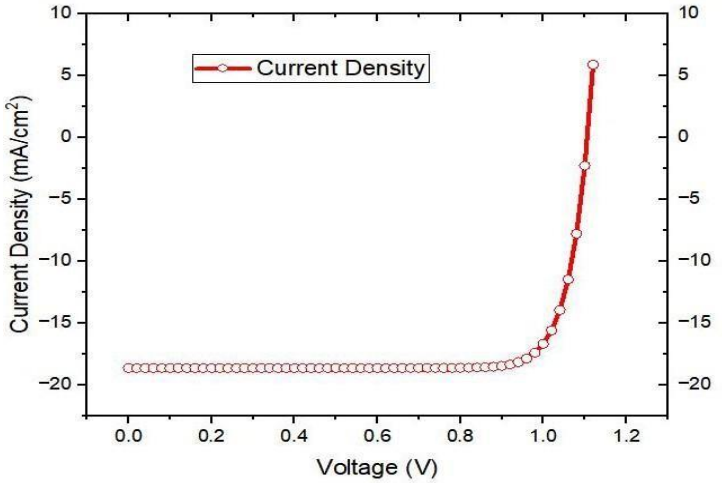

Figure 2 J–V characteristics

1) Role of Active Layer Thickness and Acceptor Density in Determining Jsc and PCE

The performance of perovskite solar cells was systematically analyzed by varying the thickness of the NiO hole transport layer (HTL) and its acceptor density. The investigation aimed to determine the influence of these two parameters on key performance metrics, specifically Jsc and PCE.

The simulation results, as illustrated in Figure 3, reveal that both Jsc and PCE increase with higher acceptor density, reaching a peak Jsc value of approximately.

18.70 mA/cm² for thinner NiO layers (around 1 μm). However, as the NiO layer thickness increases beyond 3 μm, both Jsc and PCE begin to decline. At a thickness of 5 μm, Jsc drops to 6.70 mA/cm², indicating that greater thickness leads to increased bulk resistance and recombination losses. These findings suggest that optimal performance is achieved with NiO thicknesses between 2–3 μm and acceptor densities in the range of 10^6/cm³.

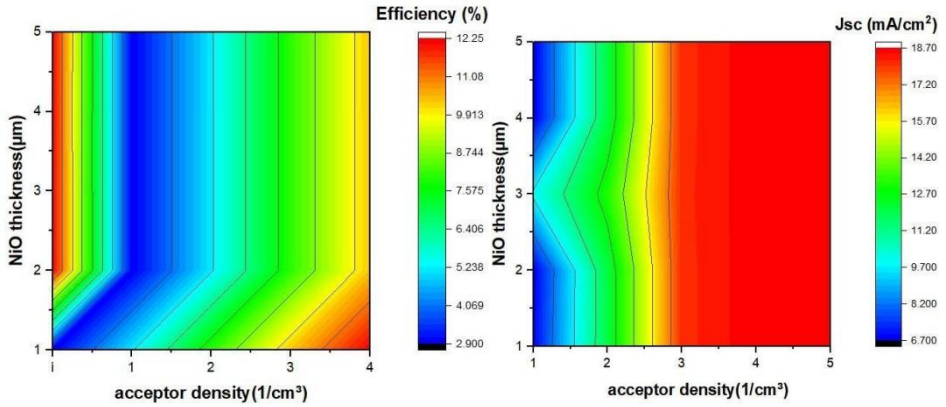

Figure 3 Jsc and PCE of NiO thickness and acceptor density

Further analysis in Figure 4 emphasizes the minor influence of ITO layer thickness ranging from 1–5 μm compared to the more dominant role of acceptor density. While a slight decrease in PCE is observed

with lower doping from 17.05% to 16.89%, the corresponding drop in Jsc is minimal, with a variation from 18.52 to 18.36 mA/cm². These results suggest that within this range, ITO thickness exerts a secondary influence on solar cell performance, while fine-tuning the acceptor density yields a modest but consistent effect.

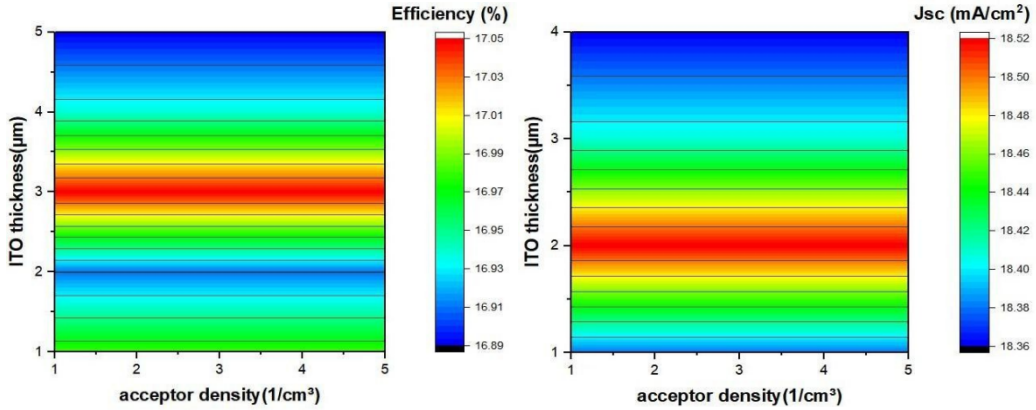

Figure 4 Jsc and PCE of ITO thickness and acceptor density

The perovskite layer, $CH_3NH_3PbI_3$, is essential for efficient light absorption and charge transport. Figure 5 illustrates the effect of varying the doping concentration in this layer. As the acceptor density decreases, both Jsc and PCE decline. Specifically, Jsc drops from 28.61 to 25.49 mA/cm², while efficiency falls from 24.35% to 22.47%, highlighting the material's sensitivity to doping. Higher doping levels improve charge carrier collection but may also increase defect density, requiring a balance to optimize performance.

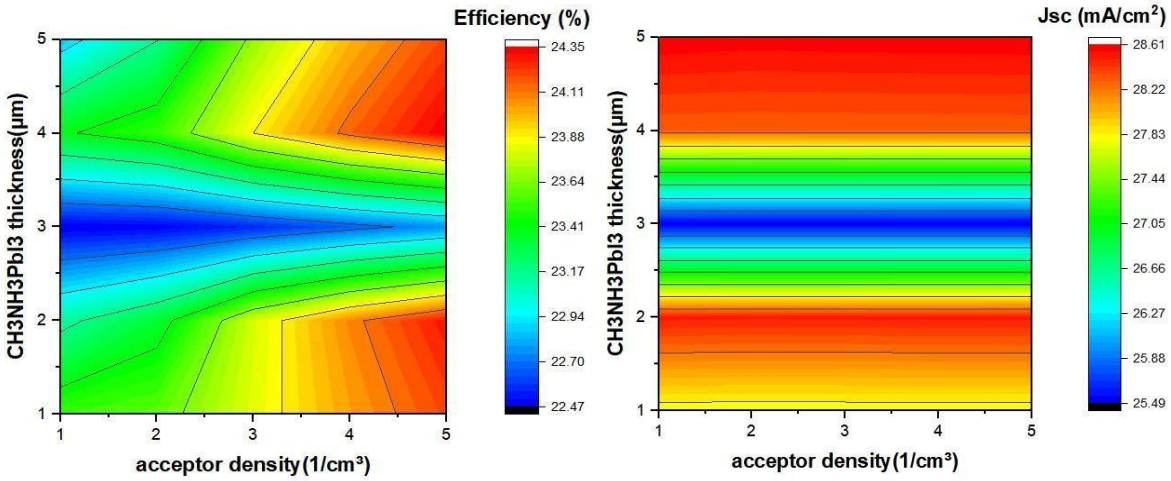

Figure 5 Jsc and PCE of Perovskite layer thickness and acceptor density

Additionally, simulations represented by Figure 6 show the influence of ZnO thickness and acceptor density on the efficiency (%) and short-circuit current density (Jsc, mA/cm²) of perovskite solar cells. Both graphs reveal minimal variation across the studied range, with efficiency consistently around 17.19–17.20% and Jsc near 18.67–18.68 mA/cm². The nearly uniform color bands suggest that within these parameters, neither ZnO thickness nor moderate doping significantly affects performance. This stability contrasts with the perovskite layer $CH_3NH_3PbI_3$, where even small changes in doping drastically affect Jsc and efficiency, making the perovskite layer much more sensitive and performance-limiting than the ZnO layer.

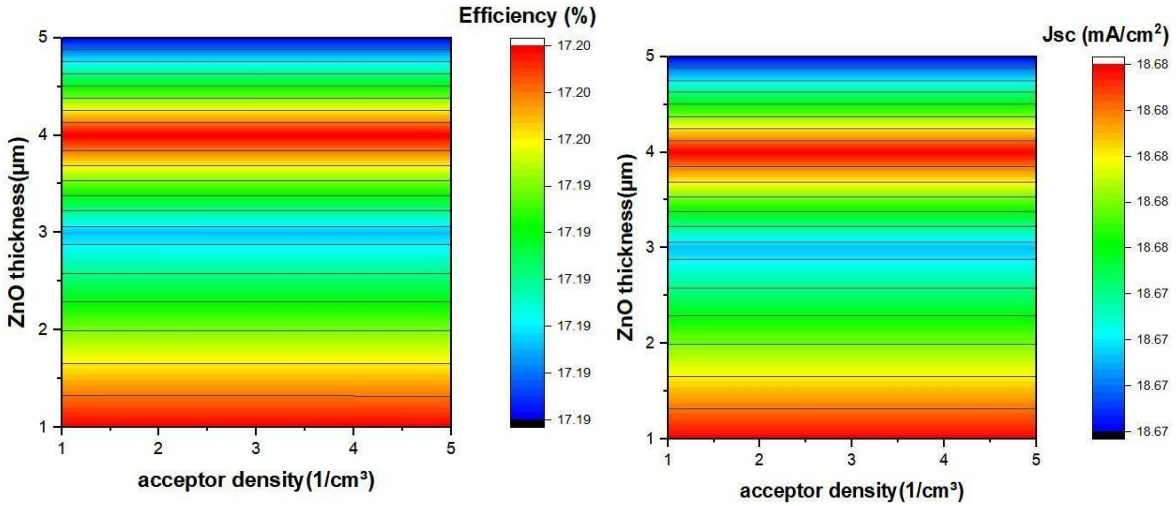

Figure 6 Jsc and PCE of ZnO layer thickness and acceptor density

Figure 7 illustrates the external quantum efficiency (QE) spectrum of the perovskite solar cell across a wavelength range of approximately 300–900 nm.

The device achieves a peak QE of around 90% near 400 nm, indicating excellent photon to electron conversion in the visible range. Efficiency remains above 80%fromabout 350 nm to 500 nm but steadily declines beyond 600 nm due to reduced absorptionandcharge collection in the near-infrared region. Below 350 nm and above 800 nm, QEdrops sharply, confirming limited response in the ultraviolet and infrared regions. This spectral behavior reflects effective light harvesting in the visible range.

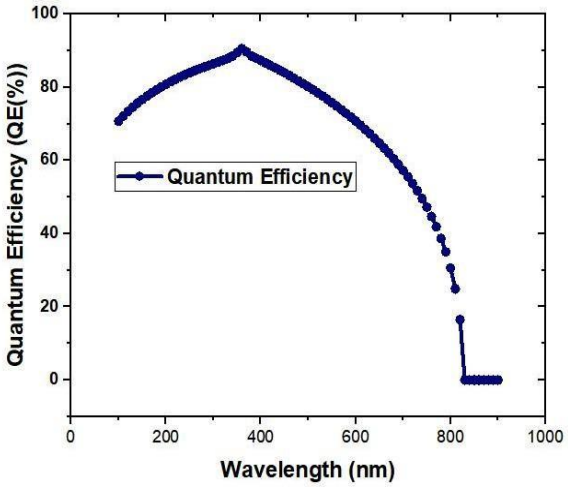

Figure 7 Quantum Efficiency

2) Influence of Thermal Effects on Performance

Figures 8, 9, and 10 collectively illustrate the thermal sensitivity of ZnOperovskite solar cells. Figure 8 presents the J–V curves of the device at various temperatures, showing that Current density slightly increases with temperature, likely due to enhanced carrier mobility. For instance, Current density improves from-18.6368824mA/cm² at 300 K to -18.6378603 mA/cm² at 350 K. However, this gain is offset byasignificant decline in open-circuit voltage (Voc), which drops from around 1.0 Vto0.8 V over the same temperature range.

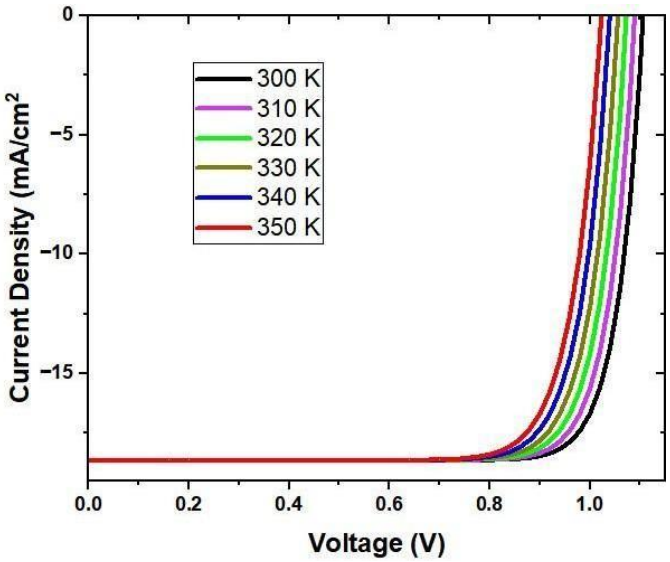

Figure 8 J-V curves with various temperature

A similar trend is observed in Figure 9, where increasing the temperature from300Kto 350 K leads to a decrease in Voc from 1.10 V to 1.02 V and in Vmpp from0.96Vto 0.866 V, indicating voltage degradation due to enhanced recombination losses. While Jsc remains nearly constant at 18.66 mA/cm², demonstrating lowtemperature sensitivity, whereas Jmpp shows a slight decrease from 17.86 mA/cm² to 17.64 mA/cm², suggesting a minor reduction in current extraction efficiency.

Figure 10 further supports this observation, showing that efficiency decreases fromapproximately 17.15% at 300 K to 15.3% at 350 K. The fill factor (FF) also declines, dropping from 83.20% to 80.21%, which further contributes to reduced overall performance. These findings highlight the critical importance of thermal stability for ensuring the practical viability and long-term reliability of PSCs in real-world conditions.

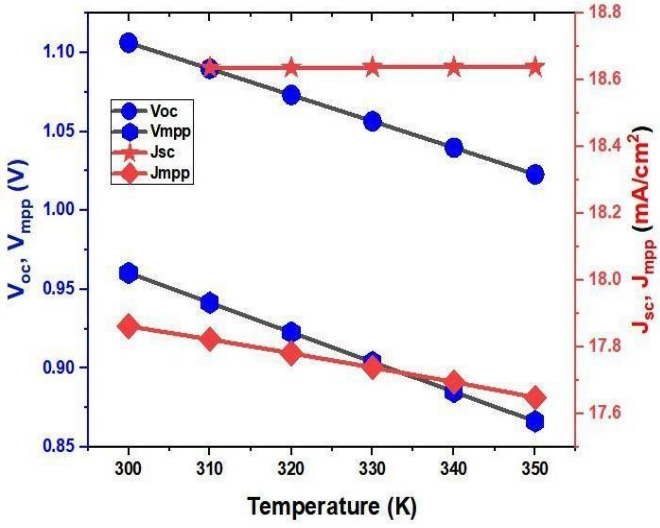

Figure 9 Voc-Vmpp and Jsc-Jmpp with temperature

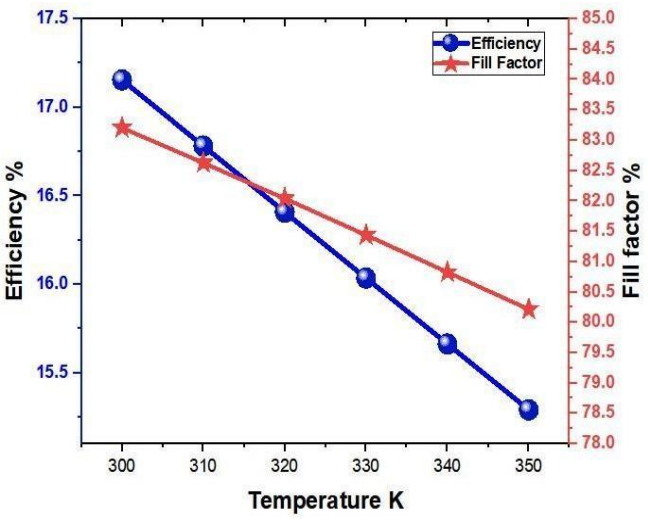

Figure 10 Efficiency and Fill factor with temperature

IV. CONCLUSION

This study demonstrates low-cost, high-performance ZnO-based perovskite solar cells using solution-processed fabrication and SCAPS-1D simulations. ZnO serves as an effective ETL due to its favorable properties, paired with $CH_3NH_3PbI_3$ and NiO layers for efficient charge transport. Optimized devices achieved 17.15% PCE with minimal recombination. NiO layer tuning significantly improves Jsc and efficiency. Thermal analysis reveals declining Voc and efficiency with temperature, emphasizing thermal

management. The approach offers a scalable, cost-effective path toward next-generation solar technologies.

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