International Journal Of Engineering Research And Development
e- ISSN: 2278-067X, p-ISSN: 2278-800X, www.ijerd.com
Volume 21, Issue 3 (March 2025), PP 207-212

Temperature-Dependent Performance Analysis of Lead-Free $MASnI_3$ Perovskite Solar Cells with Cu_2O and SnO_2 Transport Layers

Madhavi Prasangi[a]*, M.D.V. Srilalitha[b]*
[a]*Department of Freshman Engineering, Sphoorthy Engineering College, Nadergul, Hyderabad 501510, Telangana*
[b] *Department of Applied Sciences and Humanities, Maturi Venkata SubbaRao Engineering College, Nadergul, Hyderabad 501510, Telangana*
**Author for Correspondence*
(The authors have contributed equally to this work)

Abstract
In this study, the temperature-dependent performance of methylammonium tin iodide ($MASnI_3$)-based perovskite solar cells (PSCs) incorporating Cu_2O as the hole transport layer (HTL) and SnO_2 as the electron transport layer (ETL) is systematically investigated. $MASnI_3$, as a lead-free perovskite material, offers an eco-friendly alternative to lead-based counterparts, while Cu_2O and SnO_2 are chosen due to their favorable energy level alignment, high carrier mobility, and enhanced thermal stability. Current-voltage (J-V) characteristics recorded over a temperature range of 270 K to 500 K reveal a strong correlation between temperature and device performance parameters. Specifically, the open-circuit voltage (V_{oc}) decreases from approximately 1.04 V at 270 K to 0.70 V at 500 K, while the short-circuit current density (J_{sc}) shows a marginal increase. A significant decline in fill factor (FF) and power conversion efficiency (PCE) is observed, with FF dropping from 78% to 64% and PCE reducing from ~26% to 14% across the temperature range. This degradation is attributed to thermally induced non-radiative recombination, defect formation, and ion migration, which become prominent at elevated temperatures. The use of Cu_2O and SnO_2 provides better stability compared to organic HTLs and ETLs reported in earlier studies; however, the inherent thermal instability of $MASnI_3$, especially the oxidation of Sn^{2+} to Sn^{4+}, remains a critical limitation. These results highlight the importance of material engineering and interface optimization to improve the high-temperature operational stability of $MASnI_3$-based PSCs for practical photovoltaic applications.

Keywords: *$MASnI_3$ Perovskite, Temperature-dependent performance, Cu_2O Hole Transport Layer, SnO_2 Electron Transport Layer, Power Conversion Efficiency..*

Date of Submission: 15-03-2025 Date of acceptance: 31-03-2025

I. Introduction

Organic-inorganic halide perovskites have garnered significant attention over the past decade due to their remarkable optoelectronic properties and potential for low-cost, high-efficiency photovoltaic applications. Among the various perovskite materials, methylammonium tin iodide ($MASnI_3$) has emerged as a promising lead-free alternative to the widely studied lead-based perovskites, owing to its suitable bandgap (~1.3 eV), high absorption coefficient, and eco-friendly nature [1]. However, $MASnI_3$-based devices are known to suffer from intrinsic stability challenges, primarily driven by their susceptibility to oxidation and ionic defects. To overcome these limitations, recent studies have focused on optimizing device architecture, particularly the selection of appropriate electron transport layers (ETLs) and hole transport layers (HTLs), to enhance stability and efficiency [2].

Methylammonium tin iodide ($MASnI_3$) has emerged as a promising lead-free perovskite material for photovoltaic applications, owing to its suitable bandgap (~1.3 eV), high absorption coefficient, and environmentally benign composition. However, the commercialization of $MASnI_3$-based perovskite solar cells (PSCs) has been hindered by challenges related to material stability and device performance. One of the primary concerns is the susceptibility of Sn^{2+} to oxidation, leading to the formation of Sn^{4+}, which introduces deep-level defects and accelerates device degradation. To mitigate this issue, researchers have explored various strategies, including the incorporation of reducing agents and the development of oxygen-free charge transport layers. For instance, a recent study demonstrated that employing oxygen-free electron and hole transport layers can

significantly enhance the stability and performance of $MASnI_3$-based PSCs by preventing the oxidation of Sn^{2+} ions [3].

Device architecture and the choice of charge transport materials play crucial roles in determining the efficiency and stability of $MASnI_3$-based PSCs. Tin oxide (SnO_2) has been widely adopted as an electron transport layer (ETL) due to its high electron mobility, suitable band alignment with perovskite materials, and excellent optical transparency. Similarly, copper(I) oxide (Cu_2O) has emerged as an effective hole transport layer (HTL) owing to its high hole mobility, appropriate valence band alignment, and chemical stability [4]. The integration of SnO_2 and Cu_2O as ETL and HTL, respectively, has been shown to facilitate efficient charge extraction and reduce recombination losses in PSCs. However, the thermal stability of these materials and their interfaces with the perovskite absorber layer under operational conditions remains a critical area of investigation.

Temperature variations during device operation can significantly impact the performance and longevity of $MASnI_3$-based PSCs. Elevated temperatures can exacerbate ion migration, enhance defect densities, and induce phase segregation in perovskite materials, leading to performance degradation. Moreover, the thermal expansion mismatch between different layers in the device stack can induce mechanical stresses, potentially causing delamination or the formation of microcracks. Understanding the thermal behavior of $MASnI_3$-based PSCs, particularly those employing Cu_2O and SnO_2 as charge transport layers, is essential for developing strategies to enhance device stability. This study aims to systematically investigate the effect of temperature on the photovoltaic parameters of $MASnI_3$-based PSCs with Cu_2O HTL and SnO_2 ETL, providing insights into the thermal stability and guiding the design of robust, high-performance, lead-free perovskite solar cells.

Copper(I) oxide (Cu_2O) has proven to be an effective HTL in perovskite solar cells, offering advantages such as high hole mobility, appropriate valence band alignment, chemical stability, and cost-effectiveness compared to organic HTLs like Spiro-OMeTAD [4]. Similarly, tin oxide (SnO_2) is preferred as an ETL due to its superior electron mobility, wide bandgap, and low-temperature processing compatibility [5]. Prior works have demonstrated that combining Cu_2O and SnO_2 with perovskite absorbers can reduce recombination losses and improve charge extraction [6]. However, despite these material benefits, device performance is strongly influenced by environmental factors such as temperature, which can exacerbate defect formation, interfacial degradation, and ion migration in the perovskite layer and transport layers [7].

In this context, the present study focuses on systematically investigating the effect of temperature on the photovoltaic parameters of $MASnI_3$-based perovskite solar cells utilizing Cu_2O as HTL and SnO_2 as ETL. By analyzing current-voltage characteristics (JV curves) and extracting key parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and overall power conversion efficiency (PCE) at various temperatures, the stability and performance trends of these devices are elucidated. Understanding these thermal effects is crucial for evaluating the operational reliability of $MASnI_3$-based solar cells, especially for applications in flexible electronics and building-integrated photovoltaics, where devices are exposed to fluctuating temperatures. The findings offer valuable insights into thermal management strategies and optimization of transport layers to achieve thermally stable and efficient lead-free perovskite solar cells.

Numerical simulation and modeling parameters

All numerical simulations in this study were conducted using the Solar Cell Capacitance Simulator (SCAPS-1D), a widely utilized one-dimensional solar cell modeling software developed by Dr. Marc Burgelman and his research team at the Department of Electronics and Information Systems, University of Gent, Belgium. SCAPS-1D primarily functions by solving the fundamental one-dimensional semiconductor equations to accurately simulate the behavior of thin-film solar cells. Within the bulk of each layer, these governing equations include Poisson's equation alongside the carrier continuity equations (1), as outlined below, in combination with the relevant constitutive relations (2)

$$\frac{\partial n}{\partial t} = G_n - U_n + \frac{1}{q}\nabla . J_n$$

$$\frac{\partial p}{\partial t} = G_p - U_p - \frac{1}{q}\nabla . J_p$$

Where G_n and G_p are the electron and hole generation rate (cm^{-3}-s^{-1}) respectively, caused by external influences such as the optical excitation with photons or impact ionization under large electric fields. The recombination rates can be given by

$$U_n = \frac{\Delta n}{\tau_n} \text{ and } U_p = \frac{\Delta n}{\tau_p}$$

For the one-dimensional case under a low injection condition, the above equation reduce to

$$\frac{\partial n_p}{\partial t} = G_n - \frac{n_p - n_{po}}{\tau_n} + n_p \mu_n \frac{\partial E}{\partial x} + \mu_n E \frac{\partial n_p}{\partial x} + D_n \frac{\partial^2 n_p}{\partial x^2}$$

$$\frac{\partial p_n}{\partial t} = G_p - \frac{p_n - p_{no}}{\tau_p} - p_n \mu_p \frac{\partial E}{\partial x} - \mu_p E \frac{\partial p_n}{\partial x} + D_p \frac{\partial^2 p_n}{\partial x^2}$$

The above set of equations is solved numerically to extract the required solar parameters.
In the present study, One-dimensional planar n-i-p configuration (FTO/SnO_2/$MASnI_3$/Cu_2O/Au) was used for simulation by SCAPS 1D.

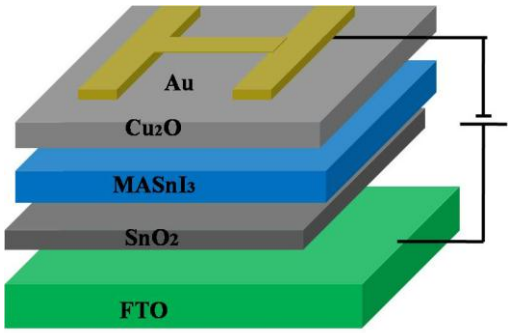

Fig. 1: Cell configuration for simulated thin film solar cell

Table 1: Input parameters of different layers used in SCAPS-1D simulation tool for the present study

Parameters	FTO	SnO_2	$MASnI_3$	Cu_2O
Thickness (nm)	400	50	500	300
Bandgap (eV)	3.5	3.2	1.3	2.17
Electron Affinity (χ)	4.0	4.0	4.17	3.2
Permittivity	9.0	9.0	6.5	7.1
Effective density of states at CB (/cm^3)	2.02E+18	1.0E+19	1.00E+18	2.5E+18
Effective density of states at VB (/cm^3)	1.8E+19	1.0E+19	1.00E+19	1.8E+19
e^- thermal velocity	1E+7	1E+7	1E+7	1E+7
h^+ thermal velocity	1E+7	1E+7	1E+7	1E+7
Mobility of e^-	2E+2	2.0E+1	1.6E+0	2.0E+2
Mobility of h^+	1E+1	1.0E+1	1.6E+0	8E+1
Density of n-type doping (/cm^3)	2E+19	1E+19	0E+0	0
Density of p-type doping (/cm^3)	0	0.0E+0	3.2E+13	9E+21
Density of defects (/cm^3)	1E+15	1E+16	1.00E+14	1E+14

II. Results And Discussion

Temperature dependent J-V curves:

The JV curves presented in fig.2 for $MASnI_3$-based perovskite solar cells, utilizing Cu_2O as the hole transport layer (HTL) and SnO_2 as the electron transport layer (ETL), clearly reveal the influence of temperature on the photovoltaic performance. At lower temperatures, specifically 270 K and 302 K, the devices demonstrate higher open-circuit voltages (Voc) around 1 V and a significant short-circuit current density (J_{sc}) exceeding 30 mA/cm². These conditions suggest minimal recombination losses, efficient charge extraction, and stable interface formation between the $MASnI_3$ absorber and the transport layers. The fill factor (FF) at these temperatures is also notably higher, indicating lower series resistance and better diode quality. As the temperature increases to 335 K and 368 K, a gradual decline in Voc is observed, likely due to the thermally activated increase in non-radiative recombination pathways. However, the current density remains relatively stable up to these intermediate temperatures, suggesting that the light absorption and carrier generation capabilities of the perovskite layer remain intact.

At elevated temperatures beyond 400 K (specifically at 434 K, 467 K, and 500 K), a marked deterioration in device performance is apparent. Both Voc and Jsc drop significantly, and the curves show increased slope in the forward bias region, indicating higher series resistance and possible degradation of charge transport layers. This behavior can be attributed to thermal instability of the $MASnI_3$ perovskite phase, ion migration, and interfacial degradation between the perovskite, Cu_2O, and SnO_2 layers. The decrease in current density suggests potential decomposition of the active layer or diffusion of elements at higher temperatures, adversely affecting carrier collection [8].

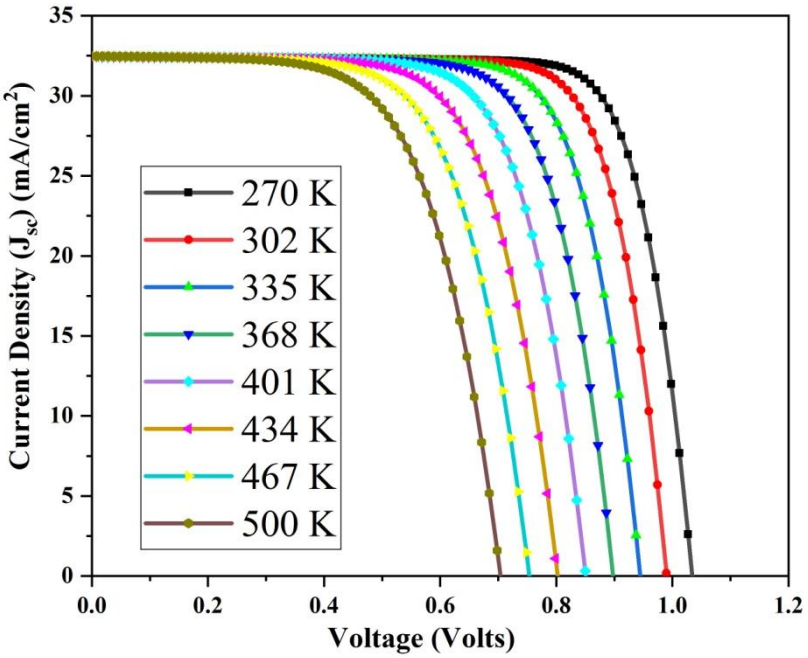

Fig. 2: J-V curves of $MASnI_3$ perovskite solar cells recorded at different temperature.

Temperature dependent Current density (Jsc) and Open circuit voltage (Voc):

The provided graph in fig. 3 illustrates the variation of open-circuit voltage (Voc) and short-circuits current density (Jsc) as a function of temperature for $MASnI_3$-based perovskite solar cells incorporating Cu_2O as the hole transport layer (HTL) and SnO_2 as the electron transport layer (ETL). It is evident that Voc exhibits a clear decreasing trend with increasing temperature, dropping from approximately 1.03 V at 270 K to around 0.72 V at 500 K. This behavior is attributed to increased thermal activation of non-radiative recombination pathways at higher temperatures, which reduce the quasi-Fermi level splitting and, consequently, Voc. Interestingly, the Jsc shows a marginal increase with temperature, rising from ~32.450 mA/cm² to ~32.470 mA/cm², suggesting that the light absorption and carrier generation remain largely unaffected or may slightly improve due to thermally enhanced carrier mobility. However, the degradation in Voc dominates overall device efficiency at elevated temperatures, emphasizing the need for better thermal management strategies.

The choice of Cu_2O as HTL and SnO_2 as ETL plays a crucial role in stabilizing charge transport and minimizing interfacial recombination losses. Cu_2O, with its high hole mobility and favorable band alignment with $MASnI_3$, supports efficient hole extraction while offering chemical stability compared to organic HTLs, as reported in literature [9]. Similarly, SnO_2 is widely recognized for its superior electron mobility, wide bandgap, and minimal hysteresis behavior, making it a preferred ETL over alternatives like TiO_2 [9]. However, despite these advantages, the thermal degradation patterns observed here highlight the limitations of the $Cu_2O/MASnI_3/SnO_2$ stack at elevated temperatures, potentially due to interface defects or ion migration. Optimizing interface passivation layers and incorporating barrier layers may mitigate these effects, making these devices suitable for applications in flexible electronics, building-integrated photovoltaics, and environments where moderate thermal fluctuations are expected.

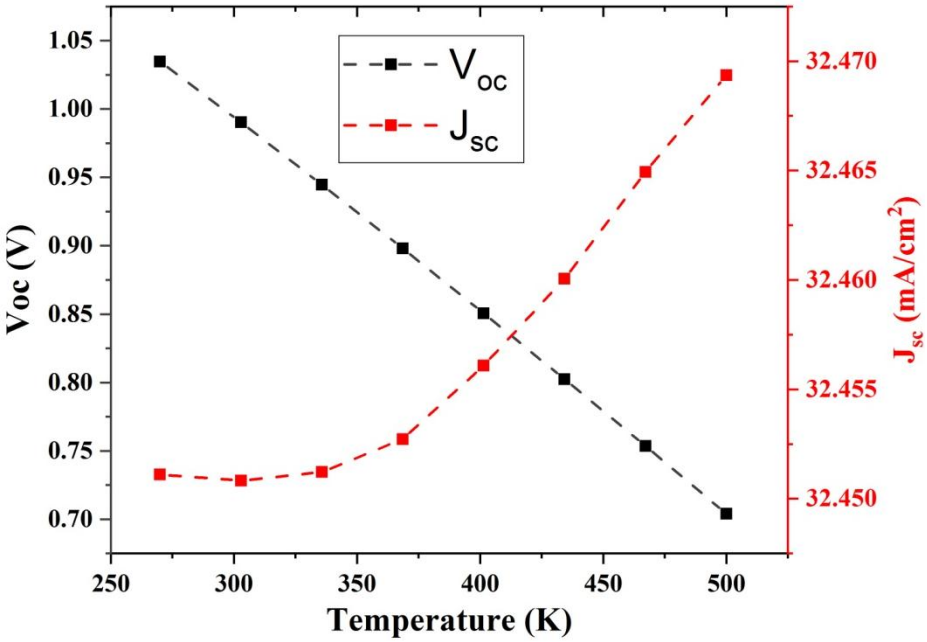

Fig. 3: Jsc and Voc of $MASnI_3$ perovskite solar cells recorded at different temperature

Temperature dependent Power Conversion Efficiency (PCE) and Fill Factor (FF):

The graph illustrates the variation of power conversion efficiency (PCE) and fill factor (FF) of $MASnI_3$-based perovskite solar cells employing Cu_2O as the hole transport layer (HTL) and SnO_2 as the electron transport layer (ETL) across a temperature range of 270 K to 500 K. A distinct decreasing trend is observed for both PCE and FF as the temperature increases. Specifically, the PCE decreases from approximately 26% at 270 K to around 14% at 500 K, while the FF drops from about 78% to 64% within the same range. This degradation is primarily attributed to enhanced recombination losses, increased defect densities, and potential thermal instability of the perovskite layer and interfacial layers at elevated temperatures. Higher temperatures are known to accelerate ion migration, especially in tin-based perovskites, which leads to non-radiative recombination pathways, adversely affecting the fill factor and overall device efficiency [10]. Additionally, thermal mismatch between layers could introduce mechanical stress and interfacial degradation, further exacerbating the decline in device performance.

The choice of Cu_2O as HTL and SnO_2 as ETL plays a critical role in influencing the thermal stability of the device. Cu_2O, with its high hole mobility, chemical stability, and favorable valence band alignment with $MASnI_3$, ensures efficient hole extraction and reduces recombination losses at the interface. SnO_2, on the other hand, offers excellent electron mobility, high transparency, and suitable conduction band alignment, facilitating smooth electron transport while minimizing energy losses. However, the effectiveness of these transport layers is also influenced by temperature variations. Previous studies have demonstrated that SnO_2 exhibits better thermal stability compared to organic ETLs like PCBM, making it more suitable for high-temperature applications. Similarly, Cu_2O has shown superior performance over conventional HTLs such as Spiro-OMeTAD due to its inorganic nature and resistance to thermal degradation [11]. Nevertheless, even with these stable transport layers, the intrinsic thermal instability of $MASnI_3$, particularly the oxidation of Sn^{2+} to Sn^{4+} at higher temperatures, remains a challenge. Therefore, understanding and mitigating temperature-induced performance losses is essential for advancing $MASnI_3$-based solar cells for real-world applications, particularly in regions with high ambient temperatures.

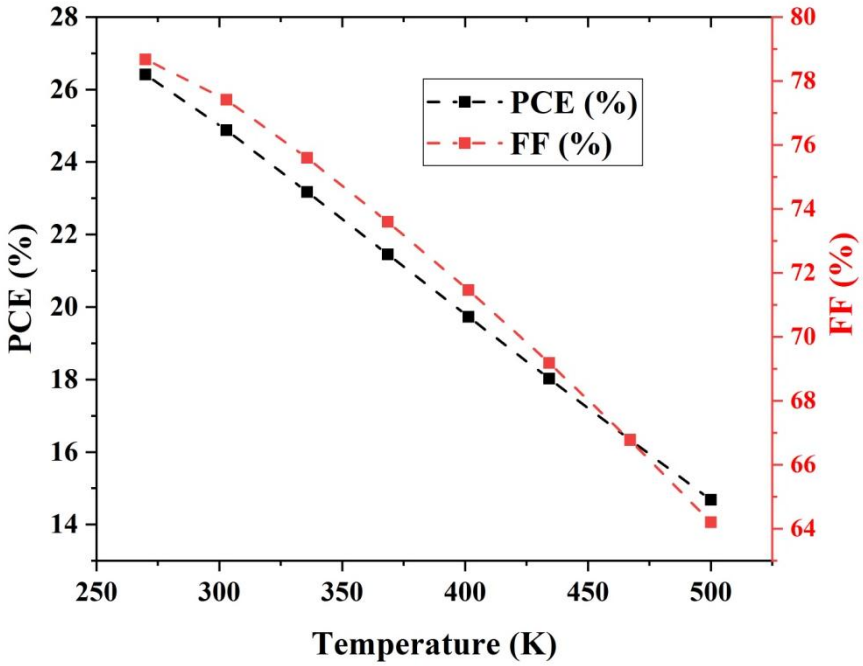

Fig. 4: PCE and FF of $MASnI_3$ perovskite solar cells recorded at different temperature

In conclusion, this study demonstrates the significant impact of temperature on the performance of $MASnI_3$-based lead-free perovskite solar cells incorporating Cu_2O as the hole transport layer (HTL) and SnO_2 as the electron transport layer (ETL). The results reveal clear temperature dependence, with power conversion efficiency (PCE) decreasing from approximately 26% at 270 K to 14% at 500 K, while the fill factor (FF) also declines from 78% to 64%. Despite these performance losses at higher temperatures, Cu_2O and SnO_2 provided better thermal stability compared to organic HTLs and ETLs, which is crucial for the development of high-temperature resilient devices. The observed decrease in open-circuit voltage (Voc) and the relatively slight increase in short-circuit current density (Jsc) at elevated temperatures suggest enhanced recombination losses and ion migration at high temperatures. These findings emphasize the importance of further optimizing the material properties of $MASnI_3$ and the interfacial layers to enhance the long-term stability and efficiency of lead-free perovskite solar cells for practical, high-temperature applications.

References

[1]. Ke, W., Stoumpos, C. C., Kanatzidis, M. G. "Unleaded Perovskites: Status Quo and Future Prospects of Tin-Based Perovskite Solar Cells." *Advanced Materials*, 31(47), 2019, 1803230.
[2]. Hao, F., Stoumpos, C. C., Chang, R. P. H., Kanatzidis, M. G. "Anomalous band gap behavior in mixed Sn and Pb perovskites enables broadening of absorption spectrum in solar cells." *Journal of the American Chemical Society*, 136(22), 2014, 8094-8099.
[3]. Noel, N. K., Stranks, S. D., Abate, A., et al. "Lead-free organic–inorganic tin halide perovskites for photovoltaic applications." *Energy & Environmental Science*, 7(9), 2014, 3061-3068.
[4]. Zhou, Y., Wang, F., Chen, Q., et al. "All-inorganic Cu_2O as a stable hole transport layer for perovskite solar cells." *Advanced Energy Materials*, 9(7), 2019, 1803244.
[5]. Ke, W., Fang, G., Wan, J., et al. "Efficient and stable perovskite solar cells using SnO_2 as electron transport layer: a review." *Journal of Materials Chemistry A*, 3(47), 2015, 23858-23870.
[6]. Bi, C., Wang, Q., Shao, Y., Yuan, Y., Xiao, Z., Huang, J. "Non-wetting surface-driven high-aspect-ratio crystalline grain growth for efficient hybrid perovskite solar cells." *Nature Communications*, 6, 2015, 7747.
[7]. Hwang, I., Jeong, I., Lee, J., et al. "Enhancing stability of perovskite solar cells to thermal stress by interface engineering." *Nano Energy*, 15, 2015, 17-27.
[8]. Zhou, Y., Wang, F., Chen, Q., et al. "All-inorganic Cu_2O as a stable hole transport layer for perovskite solar cells." *Advanced Energy Materials*, 9(7), 2019, 1803244.
[9]. Ke, W., Fang, G., Wan, J., et al. "Efficient and stable perovskite solar cells using SnO_2 as electron transport layer: a review." *Journal of Materials Chemistry A*, 3(47), 2015, 23858-23870.
[10]. Zhou, Y., Wang, F., Chen, Q., et al. "All-inorganic Cu_2O as a stable hole transport layer for perovskite solar cells." *Advanced Energy Materials*, 9(7), 2019, 1803244.
[11]. Ke, W., Fang, G., Wan, J., et al. "Efficient and stable perovskite solar cells using SnO_2 as electron transport layer: a review." *Journal of Materials Chemistry A*, 3(47), 2015, 23858-23870.