Journal of Engineering and Applied Science

Contents are available at www.jeas.ruet.ac.bd

Performance Analysis of Highly Efficient Perovskite Solar Cell Using Numerical Analysis

Sham Datto[1], Dr. Md. Faruk Hossain[2], A.R.M. Ramim[3], Md. Muhaiminul Islam[4], Anik Halder[5], Md. Maheen Mollah[6]

[1,3,4,5,6] *Department of Electronics & Telecommunication Engineering, Rajshahi University of Engineering & Technology, Bangladesh*

[2] *Department of Electrical & Electronic Engineering, Rajshahi University of Engineering & Technology, Bangladesh*

ARTICLE INFORMATION

Received date: 16 Feb 2024
Revised date: 11 May 2024
Accepted date: 24 June 2025

Keywords

Solar cell
Perovskite
HTM

ABSTRACT

Research on perovskite solar cells (PSCs) has garnered significant attention due to their potential to offer superior power conversion efficiency (PCE), cost-effectiveness, tuneable bandgap properties, low recombination rates, high open-circuit voltage (V_{OC}), ambipolar charge carrier transport, and broad-spectrum light absorption. We utilized the SCAPS-1D simulation software to optimize the performance of a PSC by employing zinc oxide (ZnO) as the electron transport layer (ETL), methylammonium tin iodide as the perovskite absorber layer, and copper iodide (CuI) as the hole transport layer (HTL). Our findings reveal that the thickness of each layer plays a crucial role in influencing the overall PCE of the PSC. Notably, the ZnO/CuI combination exhibited superior stability and degradation resistance compared to the TiO^2/CuI combination. Through optimization, we achieved a remarkable peak efficiency of 24.13%, along with a V_{OC} of 0.88 V, a J_{SC} of 37.78 mA/cm², and an FF of 72.18%. These exceptional results were attained by carefully optimizing the thicknesses of the ETL and HTL, with both achieving an ideal thickness of 400 nano meters (nm) during the final optimization stage. The optimization process underscores the promising potential of PSCs for efficient solar energy conversion. Furthermore, the improved device demonstrates stability under illumination and exhibits promising characteristics in terms of V_{OC}, J_{SC}, FF, and overall efficiency.

1. Introduction

Renewable energy has emerged as a viable option in the search for environmentally responsible and sustainable energy sources, using the strength of natural resources to satisfy our rising energy needs. Solar cells, also known as photovoltaic cells, are essential parts of renewable energy systems because they use semiconductor materials to turn sunlight into electricity. Researchers are looking into novel energy-generating technologies that could take the place of conventional solar panels and convert sunlight directly into power. Through the

provision of a more effective and sustainable source of energy, these technologies could reduce the consequences of global warming and address the energy issue [1]. Owing to its efficiency and reliability in transforming solar energy into electricity, solar cells based on silicon have served as a cornerstone in the solar energy sector for an extended period. Perovskite solar cell (PSC) has recently attracted considerable amounts of interest because of their potential to outperform conventional silicon-based solar cells in terms of performance and have remarkable photovoltaic characteristics, stability, durability, and scalability [2]. Five distinct layers constitute PSC, each of which performs a particular purpose within the cell's structure. Perovskite's structural configuration, designated as ABX_3. A-site can be occupied by various cations, including organic cations like CH3NH3+ (methylammonium) or inorganic cations like Cs+ (cesium), which can improve thermal resistance. B, on the other hand, is represented by a metal cation or a transition element, such as Pb^{2+}, and its primary function is to give catalytic activity. X stands for a halide ion, which includes compounds like iodide (I), chloride (Cl), and bromide (Br). Each ion is surrounded by eight three-dimensional structures of corner sharing octahedral elements inside the crystalline arrangement [4]. This arrangement greatly influences the properties and stability of perovskite materials.

By presenting the first PSC to the scientific community in 2006, Miyasaka and his research group achieved an important scientific milestone. Their innovative work led to the creation of a solar cell with a 2.2% efficiency rating that uses the perovskite substance $CH_3NH_3PbBr_3$ [3]. They switched from using bromine to iodine in 2009, which resulted in a significant improvement in the solar cell's efficiency, which reached 3.8% as a direct result of this modification [6]. In an effort to enhance the longevity of solar cells, Gratzel and his research team aimed to replace liquid electrolytes with solid-state organic compounds or polymers as materials facilitating hole transport (HTM). SpiroOMeTAD was used as the HTM while TiO_2 served as the electron transport material (ETM) to achieve this. In 2013, Burschka and his team achieved an efficiency of over 15% by using a TiO_2 framework and iodide deposition [8]. Later, Snaith adopted a planar assembly approach, reaching similar efficiency levels to Burschka's in the same year [9]. In 2014, Seok reported an efficiency of 17.9% by using a poly-triarylamine HTM [10]. In 2017, Seok and his research team successfully reduced defects in the perovskite layer through an intermolecular swapping approach, resulting in an impressive efficiency exceeding 22% [11]. In 2018, Agarwal and his team employed numerical simulation to design a multi-junction perovskite solar cell, achieving an impressive efficiency of 23.6% using SpiroOMeTAD type HTM [12]. In 2019, Raymond and his research group achieved the highest efficiency of 23.76% in a lead-free perovskite solar cell by utilizing Spiro-OMeTAD as the HTM [13].

The possible environmental effects of lead's presence in the perovskite absorber layer have caused serious worries. A significant barrier to the broad use of this technology has been lead toxicity, which presents dangers to human health and the environment when lead-based compounds are used in perovskite solar cells. [14].

While scientists work to develop perovskite solar cells with unprecedented efficiency (PSCs), it is imperative not to overlook the environmental consequences associated with lead. Numerous PSC configurations have been proposed to enhance efficiency while maintaining cost-effectiveness and environmental friendliness. While most studies have focused on lead-based perovskite materials, a limited number have explored alternative perovskite materials and hole transport materials (HTMs).

In our research, we employed a simulation tool known as the Solar Cell Capacitance Simulator. Utilizing actual experimental data, we integrated this simulator to analyse the behaviour and characteristics of the perovskite solar cell within our study. We have addressed the lead issue by replacing it with tin in the perovskite structure, specifically using the $CH_3NH_3SnI_3$ (methylammonium tin iodide) perovskite material. This substitution not only eliminates the environmental concerns associated with lead but also offers comparable efficiency to its lead-based counterparts. Additionally, we have employed ZnO (zinc oxide) as the hole transport material (HTM) due to its cost-effectiveness, stability, and suitable energy level alignment with the perovskite layer. Our primary motivation for this research is to develop a highly efficient and environmentally friendly perovskite solar cell solution by addressing the critical challenge of lead toxicity. We believe this can be achieved by exploring alternative materials like tin-based perovskites and cost-effective, non-toxic HTMs like ZnO.

2. Materials & Method

The Solar Cell Capacitance Simulator computer program is used to calculate the photovoltaic characteristics of solar cells. SCAPS allows for the modelling and analysis of the electrical activity of solar cells in various configurations. SCAPS-1D is a program that simulates solar cells in one dimension. Three differential equations serve as its foundation. Examples include the continuity equation for electrons and holes and Poisson's equation. Below is a display of the equations.

$$\left.\begin{aligned} q\frac{\partial n}{\partial t} &= \frac{\partial J_n}{\partial x} + qG - qR \\ q\frac{\partial p}{\partial t} &= -\frac{\partial J_p}{\partial x} + qG - qR \end{aligned}\right\} \quad (1)$$

$$\left.\begin{aligned} J_n &= qn\mu_n \frac{\partial \emptyset}{\partial x} + qD_n \frac{\partial n}{\partial x} \\ J_p &= -qn\mu_p \frac{\partial \emptyset}{\partial x} + qD_p \frac{\partial p}{\partial x} \end{aligned}\right\} \quad (2)$$

$$\frac{\partial^2}{\partial x^2}\varphi(x) = \frac{q}{\varepsilon}[n(x) - p(x) - N_D^+(x) + N_A^-(x) - p_t(x) + n_t(x)] \quad (3)$$

Where, J_n = electron current density, J_p = hole current density, p = free hole current density, q = electric charge, G = optical generation rate, R = recombination rate, $D_{n,p}$ = electron, hole diffusion coefficient, $\mu_{n,p}$ = electron, hole mobility, φ = electrical potential

A. The Device structure

The n-i-p construction is used in the proposed Perovskite solar cell (PSC) architecture. In this instance, the perovskite layer is an intrinsic layer, HTM is a p-type material, and ETM is an n-type material. Our envisioned configuration comprises a stack consisting of TCO followed by Electron Transport Material (ZnO), the absorber layer methylammonium tin iodide ($CH_3NH_3SnI_3$), and finally, the Hole Transport Material (CuI).

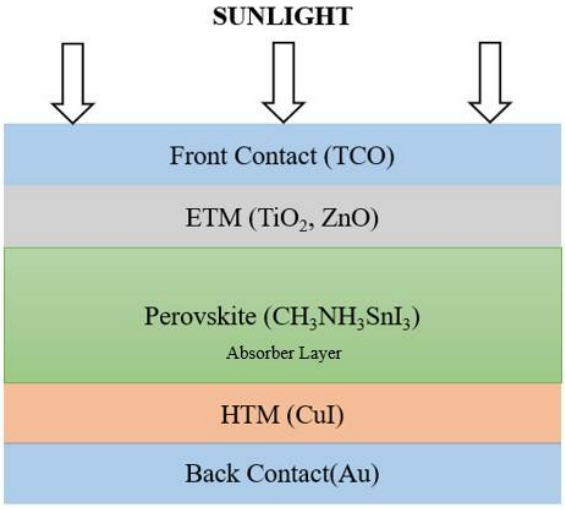

Fig. 1. Architecture of proposed perovskite solar cell

Fig. 1 depicts the cell in detail. Methylammonium tin iodide is utilized in the PSC as an absorber in between ETM and HTM. Simulated parameters for ZnO (electron transport material, ETM), $CH_3NH_3SnI_3$(absorber layer), and CuI (hole transport material, HTM) have been chosen based on a thorough review of existing literature, published experimental data, and theoretical results to ensure the robustness and credibility of our approach which is shown in Table 1 [15]. However, the series resistance (R_s) and shunt resistance (R_{sh}) will be set to appropriate values based on the chosen materials, device architecture, and typical reported values for similar devices. Sensitivity analysis will be conducted by varying R_s from lower value to higher value Ωcm² and R_{sh} from lower value Ωcm² to higher value Ωcm². The result will be valuable to understand the impact of these parameters on the simulated performance. On the other hand, the interface defect density (D_{it}) at the perovskite/charge transport layer interface will be chosen based on established models or experimental data for similar interfaces in solar cells. Sensitivity analysis will be performed by varying Dit from lower value to higher value to assess its impact on the simulated performance. The results will be also valuable to understand the influence of $D_{it.}$

The illumination spectrum employed in our study corresponds to the global AM 1.5G spectrum with an intensity of 1000 mW/cm², and we have opted for an operating temperature of 300 K as our selected condition.

TABLE I. DIFFERENT PARAMETERS USED IN THE PROPOSED PEROVSKITE SOLAR CELL FOR ANALYSIS

Material Properties	TCO	TiO_2	ZnO	$CH_3NH_3SnI_3$	CuI
X (nm)	0.500	0.050	0.050	0.400	0.050
E_g (eV)	3.500	3.200	3.300	1.300	3.400
χ (eV)	4.000	4.200	4.100	4.170	2.100
ε_r	9.000	9.00	9.000	8.200	10.000
N_C (cm^{-3})	2.000 E+18	2.000 E+18	2.000 E+18	1.000 E+18	2.000 E+18
N_V (cm^{-3})	1.800 E+18	1.800 E+19	1.800 E+19	1.000 E+18	1.800 E+19
v_n (cm/s)	1.000 E+7	1.000 E+7	1.000 E+7	1.000 E+7	1.000 E+7
v_h (cm/s)	1.000 E+7	1.000 E+7	1.000 E+2	1.000 E+7	1.000 E+7
μ_n (cm^2/V s)	2.000 E+1	2.000 E+1	1.000 E+2	1.600 E+0	2.000 E-4
μ_h (cm^2/V s)	1.000 E+1	1.000 E+1	5.000 E+1	1.600 E+0	2.000 E-4
N_D (cm^{-3})	2.00 E+19	1.000 E+16	1.000 E+16	0.000 E+0	0.000 E+0
N_A (cm^{-3})	0.000 E+0	0.000 E+0	0.000 E+0	3.200 E+15	1.780 E+17

B. Simulation Model

To analyse the perovskite solar cell (PSC), we employed the SCAPS-1D simulator. Fig. 2 and Fig. 3 display the

SCAPS-1D's layer definition panel and SCAPS-1D's material definition panel. The SCAPS 1D Layer Definition Panel refers to a component within the Solar Cell Capacitance Simulator (SCAPS) software interface. In SCAPS, this panel allows users to define the various layers that constitute the solar cell structure in a one-dimensional (1D) simulation. Users can input parameters such as layer thickness, material type, doping concentrations, mobility, and other relevant properties for each layer in the device structure. We also have taken input of different parameters which can be seen in Fig. 2.

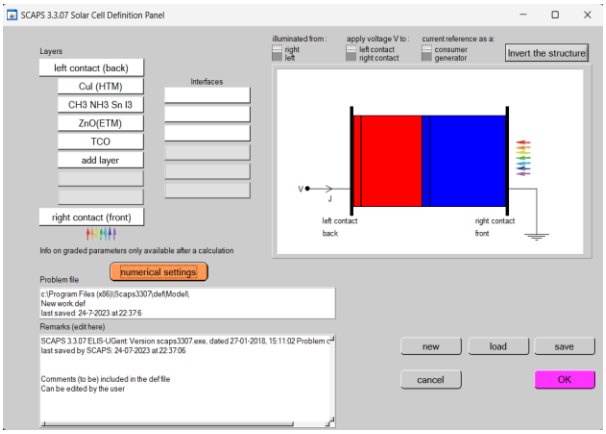

Fig. 2. SCAPS-1D layer definition model

On the other hand, the SCAPS 1D Material Definition Panel is a component within the Solar Cell Capacitance Simulator (SCAPS) software interface.

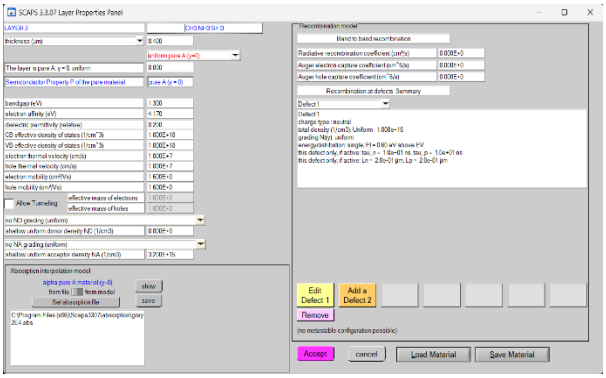

Fig. 3. SCAPS-1D material definition model

This panel allows users to define the properties of materials used in the simulation of solar cells in one-dimensional (1D) space. In the Material Definition Panel, users can input parameters related to the optical and electrical properties of materials, such as their bandgap, electron and hole mobilities, electron and hole densities, recombination rates, and interface defect densities. These parameters are crucial for accurately modelling the behaviour of solar cells under different operating conditions. The parameters can be depicted in Fig. 3. However, the working process of our simulation model in SCAPS-1D can be depicted in Fig. 4.

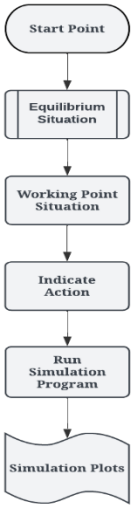

Fig. 4. Working process of our model in SCAPS-1D

However, the efficiency of solar cells is greatly influenced by recombination mechanisms, such as SRH-type, Auger, and band-to-band (direct). While Auger recombination involves the interaction of three charge carriers and the emission of a phonon, band-to-band recombination involves direct electron-hole pair annihilation. Trapping of carriers by semiconductor defects leads to SRH-type recombination. Different solar spectra are represented by illumination standards such as AM0, AM1.5D, and AM1.5G, with AM1.5G being widely used for terrestrial solar cells. The generation of electron-hole pairs and the solar spectrum are described by models such as ASTM G173 and SMARTS. The ability of a material to absorb photons is measured by the optical absorption coefficient, which is essential for figuring out the efficiency of solar cells.

3. Result and Discussion

A. Effect of Absorber Layer Thickness on Solar Cell Characteristics

Fig. 5 illustrates the intricate relationship between absorber layer thickness and four critical solar cell performance parameters. Across a thickness range of 0.1 to 1.1 µm, the V_{oc}, a measure of the maximum voltage achievable under open-circuit conditions, demonstrates

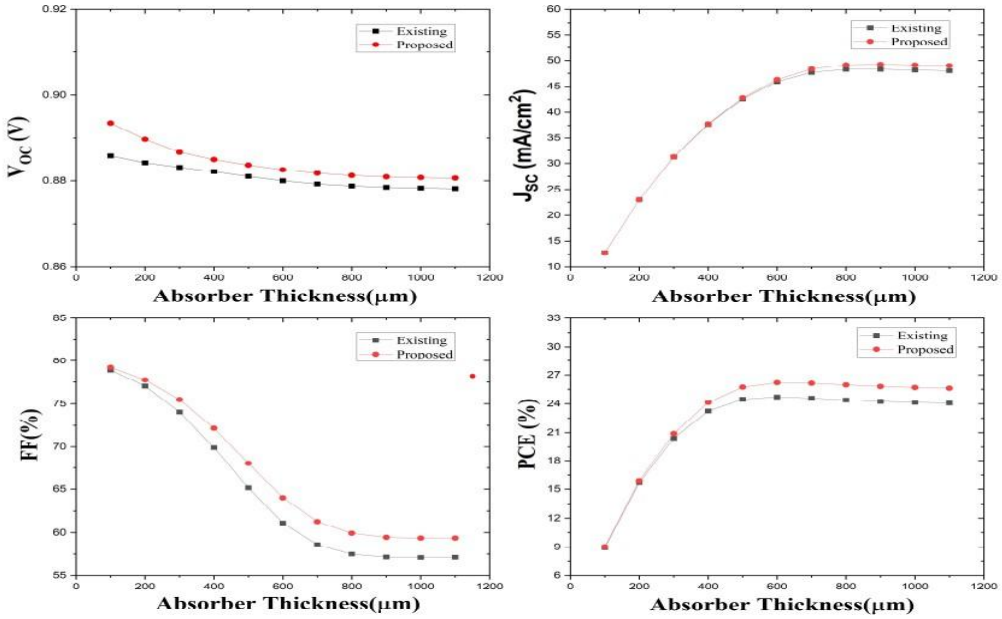

Fig. 5. Variation in photovoltaic parameters due to changes in absorber thickness.

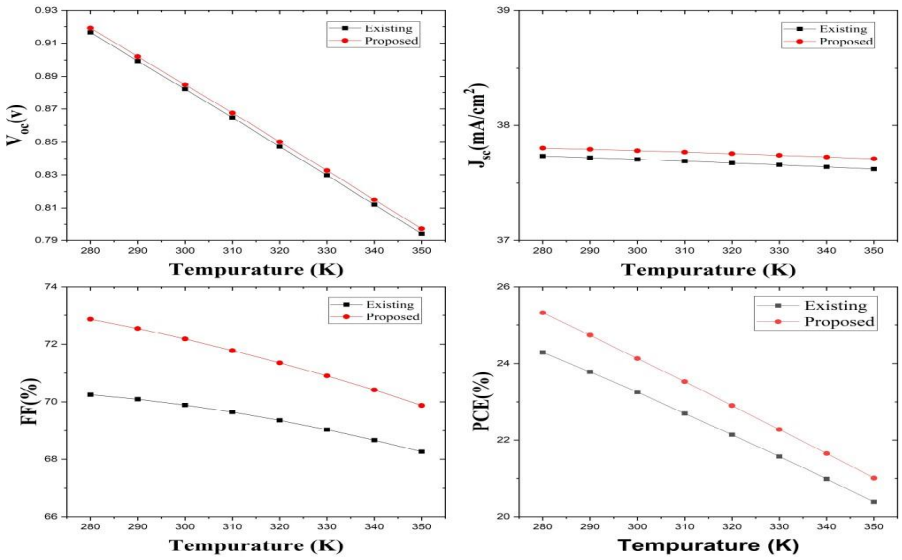

Fig. 6. Variation in photovoltaic parameters due to changes in temperature.

a consistent trend of decline as absorber layer thickness increases. This decline can be attributed to the thicker absorber layer providing more opportunities for charge carriers to recombine before reaching the electrodes. For example, as the absorber layer thickness escalates from 100 nm to 1100 nm, the V_{oc} of the current solar cell design exhibits a decrease from 0.88 V to 0.87 V. Similarly, the proposed solar cell design displays a slightly higher V_{oc} across all absorber layer thicknesses, indicating a similar behavior. Conversely, the J_{sc}, representing the maximum current achievable under short-circuit conditions, generally shows an upward trend with increasing absorber layer thickness, up to a certain threshold. This increase in J_{sc} can be attributed to the larger absorber layer's ability to absorb more photons and generate more charge carriers. However, at excessively high absorber layer thicknesses, the J_{sc} may exhibit a decline due to increased recombination and optical losses. Notably, up to a thickness of 600 nm, both existing and proposed solar cell designs experience a rise in J_{sc}, followed by a slight decline with further increases in thickness. Remarkably, the proposed solar cell design

consistently outperforms the existing design in terms of J_{sc} across all absorber layer thicknesses, likely due to its superior light absorption and charge collection capabilities. Furthermore, the Fill Factor (FF), indicative of how closely the cell's maximum power point aligns with the theoretical maximum, generally decreases as absorber layer thickness increases due to elevated series resistance. This decrease in FF is observed consistently in both existing and proposed designs. Additionally, the Power Conversion Efficiency (PCE) tends to increase with absorber layer thickness up to a certain point. This phenomenon is primarily influenced by marginal changes in V_{oc} and FF, coupled with the simultaneous increase in J_{sc}. However, at higher thicknesses, the PCE may decline due to heightened recombination and optical losses. Nevertheless, up to a thickness of 600 nm, both current and planned designs exhibit an increase in PCE, albeit followed by a slight decline afterward. The consistent outperformance of the proposed design over the existing one across all absorber layer thicknesses underscores its superiority, likely attributable to better light absorption, charge collection efficiency, and lower series resistance. It is essential to note that the performance of solar cells is significantly influenced by absorber layer thickness, with V_{oc}, FF, and PCE decreasing as J_{sc} increases up to a certain level. Additionally, it is imperative to consider the influence of temperature on these parameters, as it can also impact solar cell performance. Temperature coefficients of PV parameters should be analyzed to provide a comprehensive understanding of the proposed model's thermal stability and performance characteristics.

B. Effect of Temperature on Solar Cell Characteristics

Fig. 6 depicts the influence of temperature on key solar cell parameters: open-circuit voltage (V_{oc}), short-circuit current (J_{sc}), fill factor (FF), and power conversion efficiency (PCE). While V_{oc} generally decreases linearly and FF slightly decreases with increasing temperature due to enhanced carrier recombination and series resistance, the behavior of J_{sc} is more complex. It may exhibit a slight increase or remain relatively constant up to a certain temperature, potentially due to enhanced generation from sub-bandgap photons, before ultimately decreasing at even higher temperatures due to dominant recombination. This intricate J_{sc} behavior highlights the material-dependent nature of its temperature dependence. To comprehensively assess thermal stability, we will calculate temperature coefficients of all parameters and compare them to reported values, while also considering including a discussion on potential mechanisms influencing the observed J_{sc} behavior specific to our design. This combined analysis will provide a more nuanced understanding of our proposed solar cell's performance under varying temperature conditions.

4. Conclusion

Our study investigated the potential of lead-free perovskite solar cells (PSCs) employing copper iodide (CuI) as the hole transport layer (HTL) and zinc oxide (ZnO) as the electron transport layer (ETL). We observed a remarkable power conversion efficiency (PCE) of 24.13% for the proposed PSC when both the ETM and HTM were 0.050 µm thick [16] [17]. This finding highlights the potential of lead-free PSCs to achieve high efficiencies through careful material selection and optimization of device architecture.

Our research contributes to the ongoing search for efficient and environmentally friendly alternatives to traditional lead-based PSCs. Replacing lead with non-toxic materials like CuI aligns with the broader goal of sustainable photovoltaic technology development. It is important to note that our results surpass the PCE of 20.5% achieved by previously reported lead-free PSCs employing NiO as the HTL (Ref. [insert reference]). This comparison underscores the potential of CuI as a promising candidate for efficient hole transport in lead-free PSCs. Further studies are necessary to explore the underlying mechanisms driving the observed performance. Investigating the charge carrier transport processes at the CuI/perovskite and ZnO/perovskite interfaces, along with the impact of CuI thickness and surface modifications, could provide valuable insights for further optimization. Additionally, exploring alternative electron transport materials beyond ZnO, such as NiO, ZnS, or CdS, could offer opportunities for further performance enhancement. This research demonstrates the potential of lead-free PSCs incorporating CuI as the HTL and ZnO as the ETL to achieve high PCEs (24.13%) exceeding those of previously reported lead-free devices. This finding paves the way for further research into optimizing device architecture, exploring alternative materials, and elucidating the underlying physical mechanisms for achieving even higher efficiencies and practical implementation of these environmentally friendly solar cells.

ACKNOWLEDGMENT

The authors express their sincere gratitude to Stefaan Degrave, Marc Burgelman, Alex Niemegeers, Johan Verschraegen, and Koen Decock at Gent University in Belgium for generously granting us complimentary access to the Solar Cell Capacitance Simulator software.

References

[1] X. Zhao, C. Li, Y. Wang, W. Han and Y. Yang, "Hybridized nanogenerators for effectively scavenging mechanical and solar energies," *iScience*, Available at: www.creativecommons.org, Retrieved: May, 2021.

[2] Z. L. Wang and Z. C. Kang, "Functional and Smart Materials," Plenum Press, New York, 1998.

[3] P. Gljuscic, "NREL chart for highest confirmed conversion efficiencies for Research PV cells," *ResearchGate*. 2021.

[4] A. Kojima, K. Teshima, T. Miyasaka et al., "Novel Photoelectrochemical cell with mesoscopic electrodes sensitized by lead-halide compounds," *The Electrochemical Society*, pp. 397, 2006.

[5] A. Kojima, K. Teshima, Y. Shirai and T. Miyasaka, "Organometal halide perovskites as visible-light sensitizers for photovoltaic cells," *Journal of the American Chemical Society*, vol. 131, no. 17, pp. 6050-6051, 2009.

[6] H. S. Kim, C. R. Lee, J. H. Im, K. B. Lee, T. Moehl, A. Marchioro and M. Gratzel, "Lead iodide perovskite sensitized all-solid-state submicron thin film mesoscopic solar cell with efficiency exceeding 9%," *Scientific reports*, vol. 2, pp. 591, 2012.

[7] M. M. Lee, J. Teuscher, T. Miyasaka, T. N. Murakami and H. J. Snaith, "Efficient hybrid solar cells based on meso-superstructured organometal halide perovskites," *Science*, vol. 122, no. 8, pp. 604, 2012.

[8] J. Burschka et al., "Sequential deposition as a route to high-performance perovskite-sensitized solar cells," *Nature*, vol. 499, pp. 316-319, 2013.

[9]] S. I. Seok, M. A. Green, A. Ho-Baillie and H. J. Snaith, "The emergence of perovskite solar cells," *Nature Photonics*, vol. 8, no. 7, 2014.

[10] M. Saliba, T. Matsui, J. Y. Seo, K. Domanski, J. P. Correa-Baena, M. K. Nazeeruddin and M. Gratzel, "Cesium-containing triple cation perovskite solar cells: improved stability, reproducibility and high efficiency," *Energy and Environmental Science*, vol. 9, no. 6, pp. 1989-1997, 2016.

[11] H. Du, W. Wang and J. Zhu, "Device simulation of lead-free $CH_3NH_3SnI_3$ perovskite solar cells with high efficiency," *Chinese Physics B*, 108802, vol. 25, no. 10, Aug. 2016.

[12] E. Karimi and S. M. B. Ghorashi, "Investigation of the influence of different hole transporting materials on the performance of perovskite solar cells," *International journal for Light and Electron Optics*, vol. 130, pp. 650-658, 2017.

[13] N. Agarwal, D. Singhal, A. Kushwaha, U. Singh and B. P. Pandey, "Modelling of Multijunction Perovskite Solar Cell," *International Journal of Solid State Materials*, vol. 3, no. 1, pp. 26-31, May 2018.

[14] A. B. Coulibaly, S. O. Oyedele, N. R. Kre and B. Aka, "Comparative Study of Lead-Free Perovskite Solar Cells Using Different Hole Transporter Materials," *Modeling and Numerical Simulation of Material Science*, vol. 9, pp. 97-107, 2019. Available at: https://doi.org/10.4236/mnsms.2019.94006

[15] Coulibaly, A.B., Oyedele, S.O., Kre, N.R. and Aka, B. (2019) Comparative Study of Lead-Free Perovskite Solar Cells Using Different Hole Transpor ter Materials. Modeling and Numerical Simu lation of Material Science, 9, 97-107.

[16] Rahman, M. A. (2021). Enhancing the photovoltaic performance of Cd-free Cu2ZnSnS4 heterojunction solar cells using SnS HTL and TiO2 ETL. Solar Energy, 215, 64-76.

[17] Kumar, R. S. (2022). DESIGN AND SIMULATION OF A HIGH-PERFORMANCE CD-FREE CU2SNSE3 SOLAR CELL. NeuroQuantology, 20(18), 1554.