Research Article

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Improving Performance of Eco-friendly Perovskite Solar Cells with Fluorine Tin Oxide/Gold Nanolayers-doped Dual Optical Absorber

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ABSTRACT

Recently, perovskite solar cells are extensively studied in photovoltaics owing to their cost-effectiveness and high power conversion efficiencies. In this report, the performance of a lead-free perovskite solar cells with double optical absorbers of copper indium gallium selenide (CIGS) and methylammonium tin triiodide ($MASnI_3$) is studied using SCAPS-1D simulation. The proposed device included Spiro-OmeTAD as the electron transport layer due to its high electron mobility and suitable energy level alignment and ZnO as the hole transport layer due to its good hole mobility and good chemical stability. Fluorine-doped tin oxide and gold were used as the front and back electrode, respectively, with cadmium sulfide being used as the buffer layer. The use of p-type CIGS and $MASnI_3$ as dual absorbers enhanced light absorption and charge production, results in a power conversion efficiency of 36.4%, open circuit voltage (Voc) of 1.38 V at a fill factor of 54.2% and a short circuit current density (Jsc) of 48.3 mA/cm2. The findings demonstrate the potential of dual absorber layer engineering to enhance the efficiency of ecologically friendly perovskite solar technologies.

Keywords: Solar cells; CIGS; $MASnI_3$; Cu_2O; Spiro-omeTAD; SCAPS-1D.

1. INTRODUCTION

Currently, energy generation, energy storage, and climate change are global challenges. Increased depletion of fossil fuel reserves and high carbon dioxide emission drive the global transition to alternative energy sources and sustainability. Among these possibilities, solar energy provides a dependable solution to meet future energy requirements (Yoshikawa *et al.* 2017). Solar cell technology is significantly important to electricity generation to meet the rising demand for high-efficiency photovoltaic systems (Jiang *et al.* 2014; Hasnain, 2023). Within the next 20 years, solar energy is expected to account for up to 20% of global energy consumption. Due to its abundance, affordability, and environmental neutrality, solar energy is a smart alternative to conventional non-renewable resources worldwide with no direct impact on climate change and environmental deterioration (Liu *et al.* 2020).

Advancements in solar technologies, such as photovoltaic and thermal applications, have been attributed to more than 30 years of research and development in semiconductor-based solar technologies (Wang *et al.* 2014 and Hasnain *et al.* 2025). The most widely used commercial material for solar applications is silicon, which is preferred because of its well-characterized features (Chen *et al.* 2018). Despite efforts devoted to its development, the cost of producing ultra-pure silicon and other semiconductors do not come down. Therefore, other alternatives to replace silicon are much needed. Perovskite-structured compounds have appeared as an appealing alternative to solar energy achievement since they offer cheaper or more efficient systems.Versatile organic-inorganic perovskites have been developed for many applications, including X-ray detection systems, and have re-energized the area of sustainable energy by enabling efficient light-absorbing phases for the future development of solar cells. They provide several beneficial attributes, including strong light absorption, facile processing techniques, tunable band gaps, extended carrier diffusion lengths, and compatibility with economical, low-temperature, and solution-based deposition procedures.

According to (Shen *et al.* (2024), Ahmad *et al.* (2023), Qasim *et al.* (2022) and Kojima *et al.* (2009), the development of new generation photovoltaic materials such as perovskite materials in solar cell applications,

reported an initial power conversion efficiency of 3.8%. Since then, significant advancements have been made in both material design and engineering design, leading to a nominal power conversion efficiency (PCE) of approximately 25.5%, as reported by (Wu *et al.* 2021). However, a major impediment to the commercialization of these perovskite cells is the presence of lead in most formulations, which has raised significant concerns regarding environmental sustainability and human health. Thus, researchers are exploring lead-free approaches, utilizing various divalent metal cations such as $^{Sn2+}$ and Ge^{2+} as replacements, and they can behave similarly to Pb^{2+} and provide a safer and, more sustainable alternative.

Raj *et al.* (2021) revealed via SCAPS-based simulation that CsGeI3-based solar cells can attain a potential PCE of 18.3%. Later, they investigated other layers to achieve PCE efficiencies of 8.46% and 8.45% when depositing an electron transport layer (ETL) of SnO_2 and C60, respectively. Exploring the optimization of $CsGeI_3$ solar cell performance, (Saikia *et al.* 2022) studied how the thickness of the absorber layer, the defect density and the doping concentration resulted in variation in performance for these lead-free perovskites.

Han *et al.* (2018) presented perovskite/copper indium gallium selenide (CIGS) tandem device in which smooth surfaces for interconnecting layers with no defects found at the surface of the indium tin oxide (ITO) on which perovskite layers were deposited. By employing chemical mechanical polishing to refine the ITO surface, the researchers successfully electrodeposited perovskite layers without any degradation in device performance. This approach yielded a maximum PCE of 22.4%, along with notable enhancements in other key electrical parameters.

Jošt *et al.* (2019) also proposed an alternate fabrication process for a perovskite/CIGS tandem solar cell by growing the perovskite layer directly on the naturally textured CIGS surface, eliminating the need for the chemical polishing process. Atomic layer deposition was used to apply a thin NiOx coating on the front contact of the CIGS cell to prevent any shunting. They added a layer of poly(triaryl amine) polymer at the NiOx/perovskite interface, which contributed to a stable PCE of 21.6% due to enhanced hole transport and interface quality.

In recent years, CIGS/perovskite tandem solar cells have achieved significant experimental advancements; nonetheless, there remains substantial potential to refine critical parameters and device architecture for enhanced performance. This study carried out a comprehensive simulation-based investigation of a CIGS/$MASnI_3$ tandem photovoltaic device with the SCAPS-1D (Solar Cell Capacitance Simulator in 1 Dimension) simulator used by Bailie and McGehee (2015) to determine optimal performance conditions. The study examined temperature, interface defect density, energy band gaps, layer thicknesses, carrier generation and recombination, and doping concentrations. It also proposed and assessed a new double-junction structure based on CIGS/$MASnI_3$ with a maximum PCE of 36.38%. This emphasizes how material and interface engineering can be a useful strategy for the performance enhancement of environmentally recyclable solar cells.

2. DEVICE ARCHITECTURE

In this study, a solar cell structure based on Au/Spiro-OmeTAD/CIGS/$MASnI_3$/CdS/ZnO/FTO, was considered as presented in Fig. 1. This formation consists of materials and interfaces that are intended to be environmentally benign, while also possessing efficient charge-transport properties for enhancing photovoltaic performance. The primary contact for this arrangement is FTO, which is both transparent and conductive, allowing light entry into the device and serving as the upper electrode. The ETL of this setup is Spiro-OmeTAD, selected for its superior electron mobility and advantageous energy architecture with the absorber layers. The light-absorbing portion of the device was comprised of two absorbers (CIGS and $MASnI_3$ perovskite), to widen the absorption range and increase the amount of photogenerated carriers. ZnO was chosen as the hole transport layer (HTL) because it is an excellent hole transport material that possesses good hole mobility, offers stability in the presence of light and other factors, and is compatible with the absorbers to facilitate hole extraction. CdS was employed as a buffer layer between the absorbers and each respective transport layer, as it offers favorable optical properties and mitigates charge carrier recombination. Gold provides the rear contact for collecting holes and completes the circuit. This device structure has no lead and is comprised solely of earth-abundant materials in a manner intended to produce high efficiencies while maintaining environmental sustainability.

The fabrication of the device was simulated using the SCAPS-1D solar cell capacitance simulator, a well-established simulation tool. Material parameters for each structural layer in the device were followed as mentioned in (Singh *et al.* 2017; Zhou and Gray-Weale, 2016). A layer-by-layer approach was utilized for all possible thickness configurations. For each change, batch parameter simulations were completed, and photovoltaic performance data was recorded.

The simulation approach began by altering the thickness of the electron transport layer, ZnO, within the range 0.01 µm to 0.20 µm, and determining the thickness that yielded the optimal PCE. The thickness of the CdS layer was adjusted from 0.001 µm to 0.90 µm, and subsequently optimized for maximum efficiency. The

thickness of the light-absorbing layers were adjusted, with CH3NH3SnI3 perovskite ranging from 0.20 µm to 2.5 µm and the CIGS layer from 0.04 µm to 4.00 µm, where optimal thicknesses produced the maximum efficiency values. After stabilizing the thicknesses of the previous layers, the thickness of the HTL, Spiro-OmeTAD, was adjusted from 0.06 µm to 0.90 µm, resulting in the identification of the optimal PCE. All simulations with the SCAPS-1D simulator were performed using standard modeling procedures. The thickness measurements were obtained by the systematic technique to ensure an accurate performance assessment.

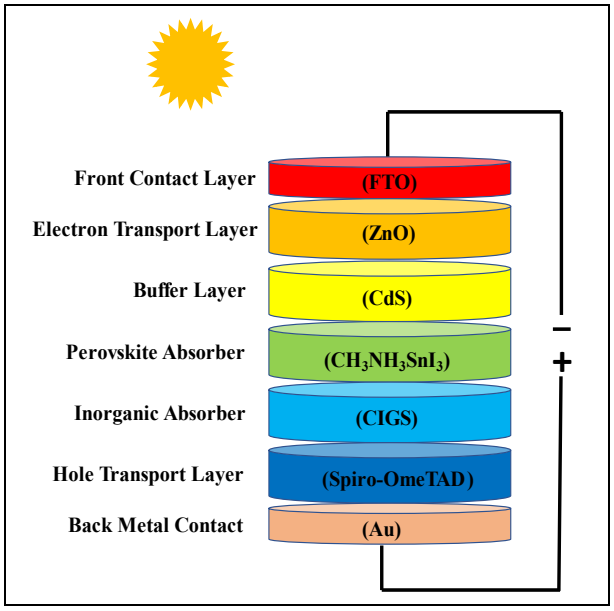


Fig. 1: Device architecture of organo-inorganic perovskite solar cell

3. RESULTS AND DISCUSSION

All layers of the device design were individually assessed in terms of their impact on overall performance. The thickness of the CIGS absorber layer was one of the most critical parameters, as seen in Fig. 2. The thickness of the CIGS layer varied from 0.08 µm to 2.1 µm, while all other layer parameters remained fixed. The goal was to determine the maximum thickness of the CIGS absorber to optimize efficiency while minimizing material use and cost. An increase in absorber thickness led to enhancements in PCE, open-circuit voltage (Voc), and short-circuit current density (Jsc). The device achieved a Voc of 1.38 V and a Jsc of 48.3 mA/cm2, resulting in a maximum efficiency of approximately 36.4%. These improvements in PEC, Voc, and Jsc are directly due to the lower recombination losses at the absorber/HTL interface and improved hole extraction, improving mobility of absorbed carriers. Remarkably, fill factor (FF) showed a small decrease with increasing CIGS absorption thickness, which means FF is less sensitive to the absorber layer thickness. Overall, increasing the thickness of the absorber resulted in noticeable gains in efficiency and reduced non-radiative losses with only a slight effect on fill factor.

Fig. 3 shows the changes in performance parameters of the $MASnI_3$-based tandem solar cell, as the $MASnI_3$ absorber thickness varies. When the $MASnI_3$ absorber thickness increases to a maximum of 2.5 µm, the FF and Jsc increase. However, PCE and Voc decrease around 0.5 µm. The highest overall device performance occurred at approximately 1.51 µm thickness, with a maximum PCE of approximately 36.4%, and Jsc and FF of approximately 48.3 mA/cm2 and approximately 54.2%, respectively. Beyond this optimum thickness, the absorber becomes thicker, leading to increased series resistance and reduced charge carrier extraction efficiency, and consequently to reduced overall performance. The findings from Fig. 3 highlight the need to thoroughly optimize the $MASnI_3$ absorber thickness to minimize resistive losses while improving charge transport for the best efficiency.

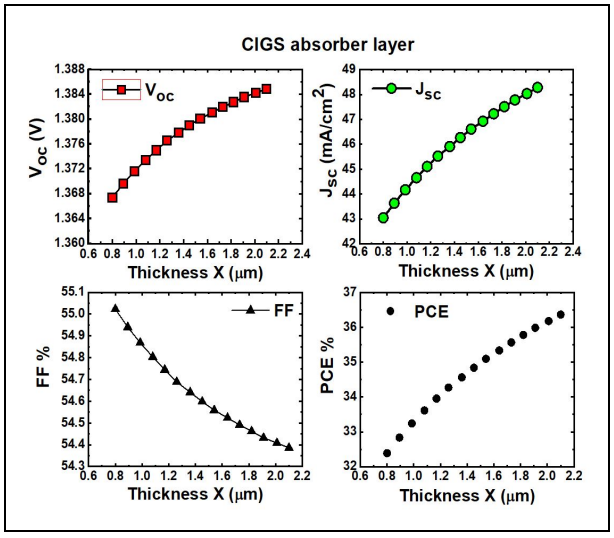


Fig. 2: Impact of thickness on efficacy of CIGS solar cell

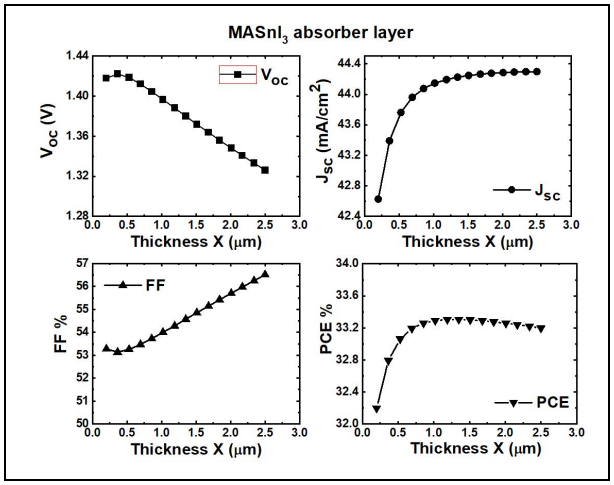


Fig. 3: Impact of the thickness on performance of $MASnI_3$ cell

The operating conditions have a major impact on efficiency of the solar cell. Using the ideal thickness values for the structural layers of the suggested cell, Fig. 4 shows the total current density (Jt) to voltage characteristics for different back-contact layers. At around 0.7 V, a noticeable increase in Jt was seen. The Jsc of 45.1 mA/cm2 was obtained at a Voc of 1.38 V. When utilizing relative humidity (Rh), a voltage breakdown took place at 0.78 V. The optimal configuration yielded a 54.2% gain in FF and a PCE of 36.4%. These results highlight the use of a back-contact material such as Au is essential for device performance in a tandem solar cells and emphasize the significance of the rear-contact layer in optimizing device efficiency.

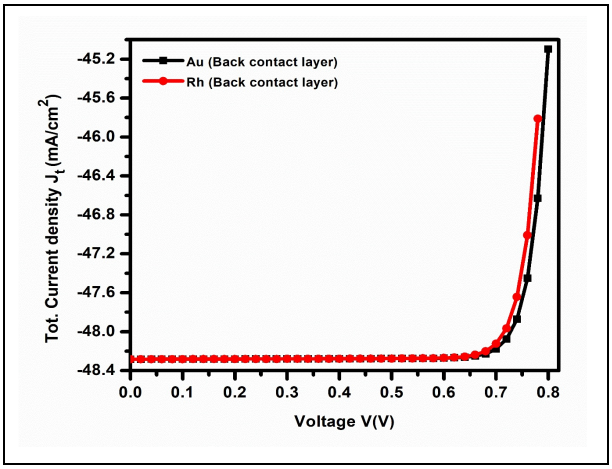


Fig. 4: Current-voltage characteristics of the proposed solar cell

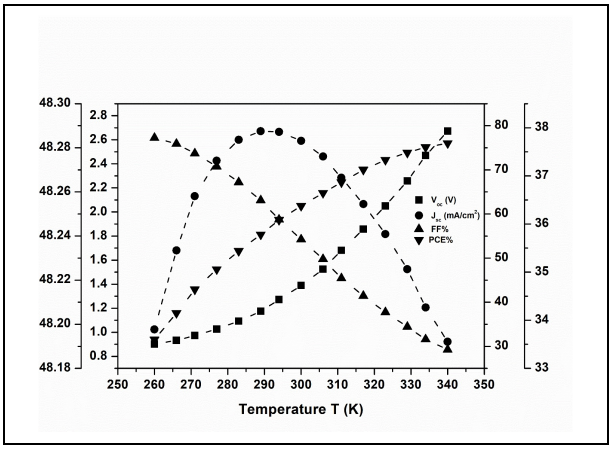


Fig. 5: Influence of temperature fluctuations on electrical performance of proposed solar cell

Variations in temperature due to sun may affect the efficiency of solar cells. Consequently, it is crucial to determine the correlation between device performance and temperature. The highlights of the working temperature curve of the proposed improved solar cell (Fig. 5) illustrate that elevated temperatures result in enhanced carrier production and improvements in the three additional electrical parameters: PCE, Voc, and Jsc. The FF exhibits a decline as temperature (T) increases. The observed loss in fill factor can be attributed to diminished device stability, thinner absorber layers, and, crucially, increased recombination and carrier lifetimes as the temperature of the CIGS/$MASnI_3$ interface increases. The result emphasizes the backdrop of heat management and material optimization to maintain sustained efficiency in devices subjected to fluctuating external circumstances.

4. CONCLUSION

This work presents an optimized solar energy harvester. To improve the performance and efficiency of the solar cell, the influence ETL and HTL inside a tandem architecture were analyzed. The ideal absorber layer thicknesses were established as 2.10 µm for CIGS and 1.51 µm for $MASnI_3$ by systematic variation. The modified design markedly improved device performance, attaining a PCE of 36.4%, a FF of 54.2%, and a Jsc of 48.3 mA/cm2. These results highlight the need to enhance the absorber layer to increase the efficiency and ecological sustainability of lead-free solar energy harvesters.

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CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

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REFERENCES

Ahmad, O., Qasim, I., Hasnain, S. M., Abdin, Z. U., Nasir, M. F., Malik, M. I. and Rashid, A., Modelling and numerical simulations of eco-friendly double absorber solar cell Spiro-OmeTAD/CIGS/$MASnI_3$/CdS/ZnO and its PV-module, *Org Electron.*, 117, 106781 (2023). https://doi.org/10.1016/j.orgel.2023.106781

Bailie, C. D. and McGehee, M. D., High-efficiency tandem perovskite solar cells, *MRS Bull.*, 40, 681-685 (2015). https://doi.org/10.1557/mrs.2015.167

Chen, Q., Wang, Y., Zheng, M., Fang, H. and Meng, X., Nanostructures confined self-assembled in biomimetic nanochannels for enhancing the sensitivity of biological molecules response, *J. Mater. Sci. Mater. Electron.,* 29, 19757-19767 (2018). https://doi.org/10.1007/s10854-018-0101-2

Han, Q., Hsieh, Y. T., Meng, L., Wu, J. L., Sun, P., Yao, E. P., Chang, S. Y., Bae, S. H., Kato, T., Bermudez, V. and Yang, A. Y., High-performance perovskite/Cu(In,Ga)Se_2 monolithic tandem solar cells, *Sci.*, 361(6405), 904-908 (2018). https://doi.org/ 10.1126/science.aat5055

Hasnain, S. M., Examining the advances, obstacles, and achievements of tin-based perovskite solar cells: A review, *Sol. Energy.*, 262, 111825 (2023). https://doi.org/10.1016/j.solener.2023.111825

Hasnain, S. M., Iqbal, A., Qasim, I., Irshad, K., Mir, M. A., Malik, M. I. and Sundar, L. S., Performance evaluation of organometal halide $MASnI_3$ and inorganic $BaZrS_3$ hybrids in perovskites solar cells: Theoretical approach, *Hybrid Adv.*, 9, 100408 (2025). https://doi.org/10.1016/j.hybadv.2025.100408

Jiang, T., Wang, Y., Meng, D., Wu, X., Wang, J. and Chen, J., Controllable fabrication of CuO nanostructure by hydrothermal method and its properties, *Appl. Surf. Sci.*, 311, 602-608 (2014). https://doi.org/10.1016/j.apsusc.2014.05.116

Jošt, M., Betram, T., Koushik, D., Marquez, J. A., Verheijen, M. A., Heinemann, M. D., Kohnen, E., Ashouri, A. A., Braunger, S., Lang, F., Rech, B., Unold, T., Creatore, M., Lauermann, I., Kaufmann, C. A., Schlatmann, R. and Albrecht, S., 21.6%-efficient monolithic perovskite/Cu(In,Ga)Se_2 tandem solar cells with thin conformal hole transport layers for integration on rough bottom cell surfaces, *ACS Energy Lett.*, 4(2) 583-590 (2019). https://doi.org/10.1021/acsenergylett.9b00135

Kojima, A., Teshima, K., Shirai, Y. and Miyasaka, T., Organometal halide perovskites as visible-light sensitizers for photovoltaic cells, *J. Am. Chem. Soc.*, 131(17) 6050-6051 (2009). https://doi.org/10.1021/ja809598r

Liu, J., Chen, K., Khan, S. A., Shabbir, B., Zhang, Y., Khan, Q. and Bao, Q., Synthesis and optical applications of low dimensional metal-halide perovskites, *Nanotechnol.*, 31(15), 152002 (2020). https://doi.org/10.1088/1361-6528/ab5a19

Qasim, I., Ahmad, O., Abdin, Z. U., Rashid, A., Nasir, M. F., Malik, M. I., Rashid, M. and Hasnain, S. M., Design and numerical investigations of eco-friendly, non-toxic (Au/CuSCN/$CH_3NH_3SnI_3$/CdTe/ZnO/ITO) perovskite solar cell and module, *Sol. Energy.*, 237, 52-61(2022). https://doi.org/10.1016/j.solener.2022.02.056

Raj, A., Kumar, M., Bherwani, H., Gupta, A. and Anshul, A., Evidence of improved power conversion efficiency in lead-free $CsGeI_3$ based perovskite solar cell heterostructure via scaps simulation, *J. Vac. Sci. Technol. B.*, 39(1), 012401(2021). https://doi.org/10.1116/6.0000718

Saikia, D., Bera, J., Betal, A. and Sahu, S., Performance evaluation of an all inorganic CsGeI3 based perovskite solar cell by numerical simulation, *Opt. Mater.*, 123, 111839 (2022). https://doi.org/10.1016/j.optmat.2021.111839

Shen, Y., Ran, C., Dong, X., Wu, Z. and Huang, W., Dimensionality engineering of organic–inorganic halide Perovskites for next-generation X-ray detector, *Small.*, 20(16), 2308242 (2024). https://doi.org/10.1002/smll.202308242

Singh, N., Chaudhary, A.K., Saxena, S.K., Saxena, M. and Rastogi, N., Electrical simulation of organic solar cell at different charge carrier mobility, *IOSR J. Appl. Phys.*, 09(02), 01-04 (2017). https://doi.org/10.9790/4861-0902020104

Yoshikawa, K., Kawasaki, H., Yoshida, W., Irie, T., Konishi, K., Nakano, K., Uto, T., Adachi, D., Kanematsu, M., Uzu, H. and Yamamoto, K., Silicon heterojunction solar cell with interdigitated back contacts for a photoconversion efficiency over 26%, *Nat. Energy*, 2, 17032(2017). https://doi.org/10.1038/nenergy.2017.32

Wang, Y., Jiang, T., Meng, D., Yang, J., Li, Y., Ma, Q. and Han, J., Fabrication of nanostructured CuO films by electrodeposition and their photocatalytic properties, *Appl. Surf. Sci.*, 317, 414-421 (2014). https://doi.org/10.1016/j.apsusc.2014.08.144

Wu, J., Li, Y., Yiming, L., Xie, W., Shi, J., Li, D., Cheng, S. and Meng, O., Using hysteresis to predict the charge recombination properties of perovskite solar cells, *J. Mater. Chem. A.*, 9(10), 6382-6392 (2021). https://doi.org/10.1039/D0TA12046D

Zhou, Y. and Gray-Weale A., A numerical model for charge transport and energy conversion of perovskite solar cells, *Phys. Chem. Chem. Phys.*, 18(6), 4476-4486 (2016). https://doi.org/10.1039/C5CP05371D