Eurasian Journal of Science and Technology

2024, Volume 4, Issue 3

Original Article

Enhanced Solar Cell Efficiency with Tin-Based Lead-Free Material ($FASnI_3$) through SCAPS-1D Modeling

Ateeq ul Rehman[1] | **Tahir Munir**[1, 2] | **Shahbaz Afzal**[2, 3] | **Muhammad Saleem**[1] | **Imosobomeh L. Ikhioya**[2, 4,*]

[1]*Institute of Physics, Baghdad ul Jadeed Campus, The Islamia University of Bahawalpur, Bahawalpur 63100, Pakistan*
[2]*National Centre for Physics, Quaid-i-Azam University Campus, Islamabad, 44000, Pakistan*
[3]*Department of Physics, University of Education Lahore, DG Khan Campus 32200, Pakistan*
[4]*Department of Physics and Astronomy, University of Nigeria Nsukka, 410001, Nigeria*

Use your device to scan and read the article online

Citation A.U. Rehman, T. Munir, S. Afzal, M. Saleem, I.L. Ikhioya, **Enhanced Solar Cell Efficiency with Tin-Based Lead-Free Material ($FASnI_3$) through SCAPS-1D Modeling.** *Eurasian J. Sci. Technol.*, **2024**, *4*(3), 244-252.

https://doi.org/10.48309/EJST.2024.429200.1118

Article info:
Received: 2023-12-06
Accepted: 2024-01-28
Available Online: 2024-02-12
ID: EJST-2401-1118
Checked for Plagiarism: Yes
Checked Language: Yes

Keywords:
Perovskite Solar Cells (PSC), $FASnI_3$, HTL, Thickness, Acceptor Density NA.

ABSTRACT

Recent successes in the development of lead (Pb) halide perovskites have urged extensive research into cost-effective photovoltaic devices, to avoid significant challenges related to stability and toxicity. In this study, device modeling was presented for lead (Pb)-free perovskite solar cells (PSC), by employing $FAsnI_3$ as the perovskite absorber layer. The simulation evaluates the impact of varying thickness, acceptor density of the hole transport layer (HTL), and temperature within the ranges from 50 to 250 nm, $1x10^{18}$ cm^{-3} to $1x10^{22}$ cm^{-3}, and 300 K to 450 K, respectively. The photovoltaic cell has inverted geometry (p-i-n) and device structure is ITO/PEDOT:PSS/$FASnI_3$/BCP/Au. The $FASnI_3$-based PSC exhibits an efficiency of 14.03%, current density (Jsc) 20.4 mA/cm^2, fill factor (FF) 76.7%, and open circuit voltage (Voc) 0.92 V and these results are already presented experimental with same device structure. These results showed that a more eco-friendly solar cell using methyl ammonium tin was created successfully as perovskite. It is suggested to use alternative materials instead of methyl ammonium tin as perovskite.

Introduction

The perovskite solar cells (PSC) which are based on the halide-lead are those solar cells which have an efficiency which is like the silicon based solar cells. In the future, they will compete the conventional solar cells, because they have favorable light absorption, excellent lifespan, variable absorption coefficients, extended diffusion length, simple production procedures, and other advantages [1,2]. PSC with the $MAPbI_3$ gave an efficiency up to 25.7% which was starting from a very small number 3.8%. This increase in an efficiency noticed in a very short duration [3,4]. Beside that there are lot of problems related to the use of lead based perovskite materials, because these materials

---

**Corresponding Author: Imosobomeh L. Ikhioya. imosobomeh.ikhioya@unn.edu.ng* are lead toxic which effect the environmental factors [5]. Accordingly, many researchers are moving towards the lead free PSC, using the Sn/Ge and Bi/Sb for the assembling of lead free PSC with 1.41 to 1.21 band gap, non-toxic effect, larger electrical response, and good stability [6-10]. The lead free and lead based perovskite solar cells both nearly show same efficiency [11,12]. Whereas thermal stability of FA is larger than that of MA so there is other need to be replacing MA by FA in PSC and Pb with Sn. The new perovskite material $FASnI_3$ came which have lower band gap (Eg) 1.41 and large temperature stability about 200 °C, due to that reasons this perovskite material get an attraction by the researcher's and many of research has been done on it with the power conversion efficiency from 2.1% to 14% experimentally according to our literature survey [13,14]. When we use $FASnI_3$ as a perovskite layer then, overall size of the film will increase and cause the maximum light harvesting [15,16], where Abdelaziz *et al.* use the SCAPS-ID simulation software to notice the effect of different factors on performances of the $FASnI_3$ based solar cells like thickness, donor density, defect density, doping concentration and an efficiency of the cell up to 14.3% [17-19].

This study aims to improve solar cell efficiency using tin-based lead-free material (FASnI3) with SCAPS-1D modeling. In our inverted solar cell with p-i-n geometry, $FASnI_3$ was utilized as a perovskite material and simulate the experimental work under AM1.5G light. The process can be simulated at a temperature of 300k by adding a maximum of seven sheets, in both dark and light environments. Aggregate and interface imperfections can have permitted concentrations. It can be used with both amorphous and crystalline photovoltaic panels.

Simulation Parameters

PSC structure is constructed as hole and electron transport layers are known as HTL and ETL, transparent glass (FTO and ITO), in addition, perovskite layer (absorber layer) is presented between the HTL and ETL, as displayed in Figure 1 [19]. Depending on the arrangement of layers, PSC have two different types of geometry planer (n-i-p) and inverted (p-i-n). An electrons and holes are extracted from the absorber layer and move toward the respective layer like ETL and HTL [20,21]. Our solar cell is inverted in which the arrangement of the layers is ITO/ PEDOT:PSS/ $FASnI_3$/ BCP/Au. In our cell, PEDOT:PSS acts as the HTL, $FASnI_3$ behaves like a PAL and indene-C_{60} bisadduct (ICBA) BCP is ETL. Geometry of the presented solar cells is same as the experimental one [7]. Some parameters data is from already presented simulation works, which we use for our simulation in Table 1 [17,22]. The power conversion efficiency was noticed from the simulation work is related to the experimental work which is already done by Zhu *et al.* [23].

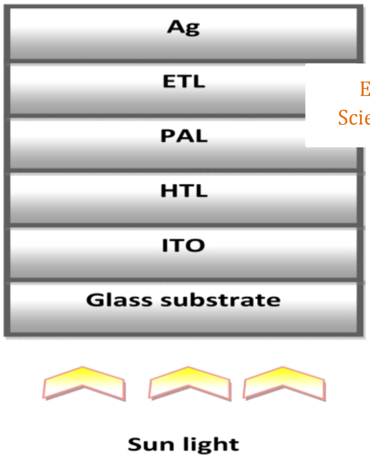

Figure 1 Perovskite solar cell [24]

Results and Discussion

In this section, some factors are discussed affecting on the resultant efficiency like thickness, donor density of HTL, and the temperature by the SCAPS-1D simulation software.

Effect of Thickness of Hole Transport Layer

The efficiency of photovoltaic cells is significantly influenced by the HTL. Here, we observed the effect of increasing the HTL thicknesses between 50 nm to 250 nm upon the efficiency of the photovoltaic cell, as depicted in Figure 2(a-d).

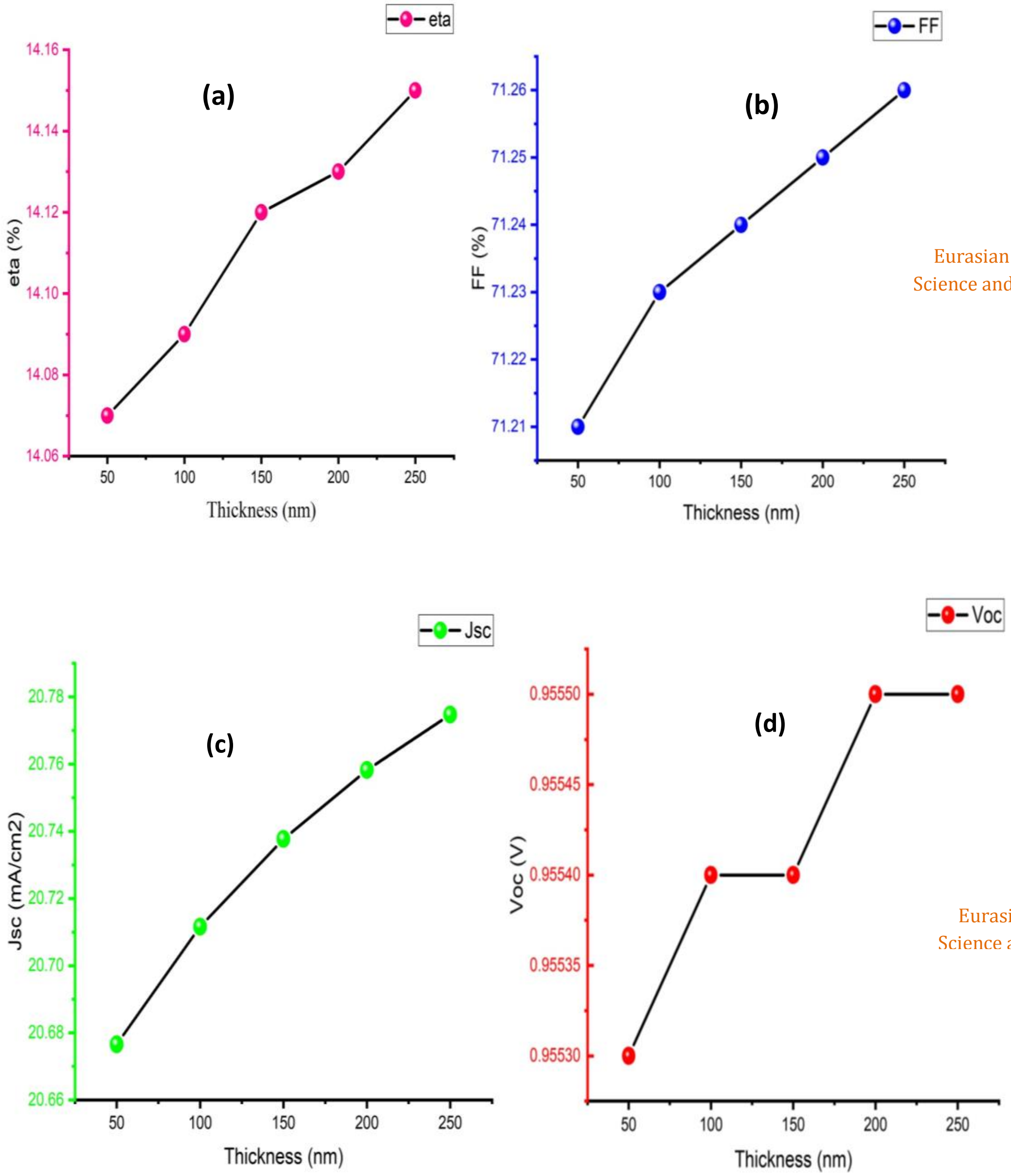

Figure 2 (a) Effect of HTL thickness on PEC and (b) effect of HTL thickness on Fill factor(c) Effect of HTL thickness on Jsc and 2(d) Effect of HTL thickness on Voc

Initially, Figure 2 (a) shows, when the thickness were increases from 50 nm to 250 nm with the gap difference of 50 nm, PCE of device was decreased between 14.07% and 8.38%, respectively. When the HTL thickness was increased, the hole movement was decreased from layer to glass and reason recombination was increased in the film.

Table 1 Parameters used for simulation [17,22]

Parameters	**ITO**	**PEDOT:SS**	**FASnI$_3$**	**BCP**
NA(cm^{-3})	0 [25]	0	0	1.0E+18
ND(cm^{-3})	1.0E+21 [25]	1.0E+18	7.00E+16	0
Hole-mobility (cm^2/Vs)	1.0E+1 [25]	4.50E-2	2.2E+1	8.600E+3
Electron-mobility (cm^2/Vs)	2.0E+1	4.50E-2	2.2E+1	2.0E+2
VB (cm^{-3})	1.8E+19	1.8E+19	1.0E+18	1.0E+19
CB (cm^{-3})	2.2E+19	2.0E+18	1.0E+18	2.0E+19
Permittivity	9.00	3	8.200	7.5
Band gap (eV)	3.5	1.6	1.41	2.2
Thickness (nm)	500	50	350	50
Electron affinity (eV)	4.0	3.9	4.0	3.4

When the thickness of HTL rises, fill factor falls, as Figure 2 (b) illustrated. The main reason in the decreasing the value of Fill factor is increased in resistance of the device. This is because the thicker layer limits the carriers' mobility, leading to a decrease in the current density and a decrease in the device efficiency. In addition, the thicker layer increases the surface states, result higher surface recombination and decline the number of charge carriers reaching in the electrodes. Due to the reason of these factors FF decreases in Table 2 [26,27].

From Figure 2 (c), it is noticed that the current density values are further decreased because due to increased recombination [28]. Likewise, the charge carriers towards the electrodes decrease, leading to a fall in current density. Figure 2 (d) illustrates that the Voc (open circuit voltage) decreases because when thickness of layer increases, there is a greater distance for the photogenerated electrons and holes to travel before they reach their respective electrodes, leading to more recombination, and recombination of carrier consequences in a decrease in Voc [29].

Effect of Acceptor Density (NA) of Hole Transport Layer

Acceptor density shows an energetic role in enactment of photovoltaic cell. Here, we increase value of acceptor density to notice its effect on enactment of device, while other parameters of layers will remain optimize.

Table 2 Comparisons of simulation work with experimental

Parameters	**ITO/PEDOT:SS/FASnI$_3$/BCP**	**ITO/PEDOT:SS/FASnI$_3$/BCP**
PEC (%)	14.03	14.07
Jsc (mA/cm^2)	20.4	20.67
Voc (V)	0.92	0.95
FF (%)	76.7	71.21
Referances	Experi. [23]	Simulation

The performances of photovoltaic cell were increased by increasing the acceptor density as shown in Figure 3 (a-d). Figure 3(a) demonstrates that efficiency of the cell increases from 14.07% to 14.21%, when the acceptor density increases from 1x10^{18} to 1x10^{22}, because the mobility of charge carriers are increased and they are able to reach their respective electrode. The increased in mobility of charge carriers is due to increased number of available dopant molecules/ions with higher acceptor density. These dopant molecules/ions act as charge carriers, enabling the transport of electric charge through the material and become the main reason in increasing the cell efficiency [30,31].

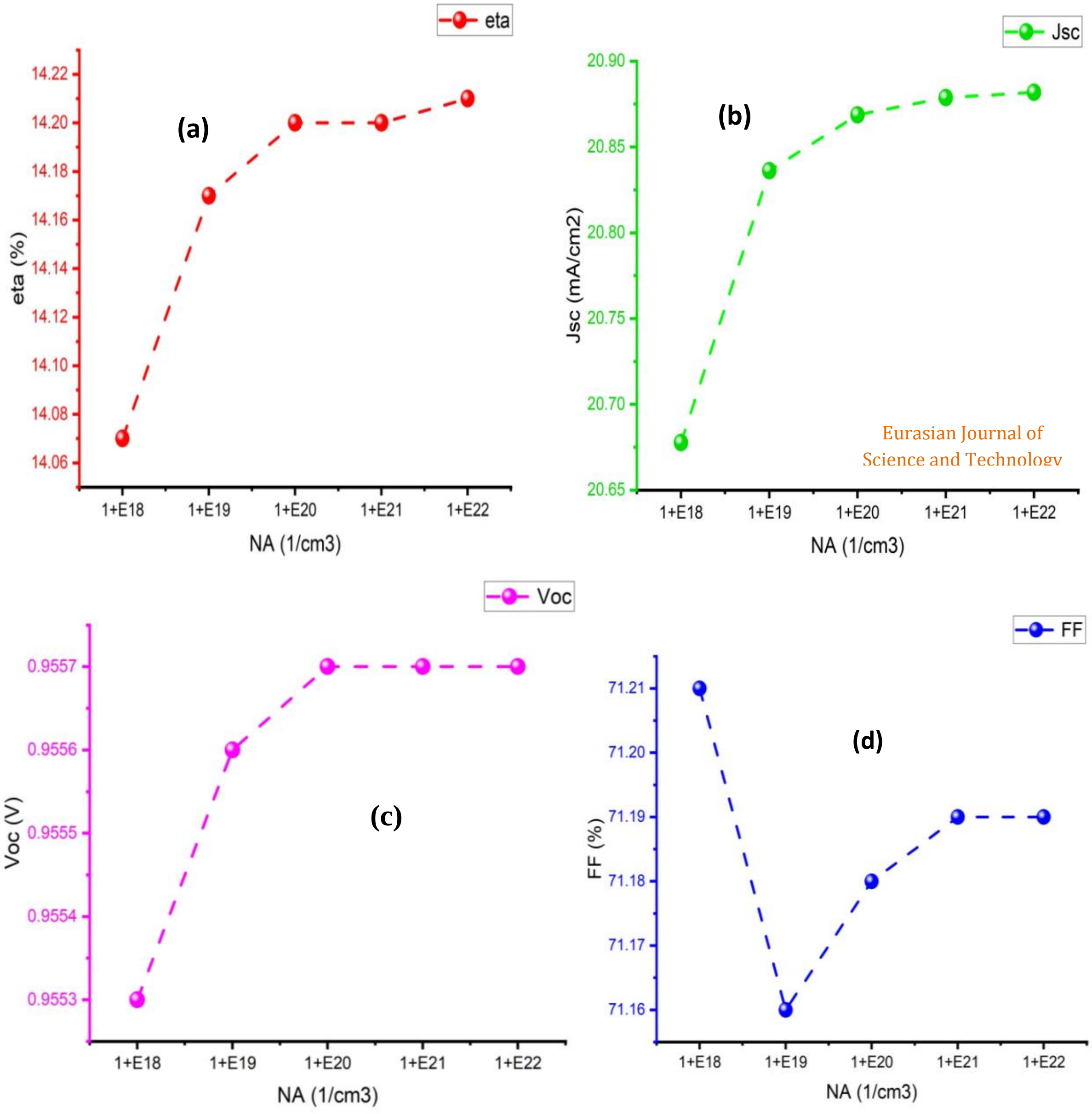

Figure 3 (a) Effect of HTL acceptor density on PCE, (b) Effect of HTL acceptor density on Jsc, (c) Effect of HTL acceptor density on Voc, and (d) Effect of HTL acceptor density on FF

While the current density values are increases from 20.6776 mA/cm^2 to 20.8818 mA/cm^2 as illustrate in Figure 3(b). This is due to decrease in resistance within the structure of the device while Voc is not affected as we can see in Figure 3 (c), because V_{OC} is depended on band gap of semiconductor material, which is not changed by the increased acceptor density [32]. Fill factor

(FF) of PSC is playing a vital role that describes the cell competence in converting sunlight into electrical energy, and which is ratio of the power maximum output of cell to the product of Voc and Jsc. The FF of a PSC can be affected by different factors, such as the recombination rates of charges, movement of charges, and the electrical conductivity of the different layers in the device [33]. Figure 3(c) shows the effect of acceptor density on FF, when NA of HTL increases from 1×10^{18} to 1×10^{22}, this leads to a complex interplay between charge collection efficiency and recombination rates, resulting in a small increase in the FF of the PSC.

Effect of Temperature on Device Performance

The PSC performance was decreased significantly, as shown in Figure 4 (a-b) whereas the efficiency, FF, Jsc, and Voc values remained from 14.07 % to 9.51 %, 71.21 % to 64.83 % , 20.6776 mA/cm^{3} to 22 0.75475 mA/cm^{3}, and 0.9553 V to 0.6646 V, when the system temperature increases from 300 k to 500 k. This decrease in performance is mainly due to changes in the bandgap, charge carrier mobility, crystalline structure, and device stability.

***Bandgap Narrowing*:**PSC have an E_g between 1.5-1.6 eV, which means that it can absorb photons in the visible range. However, when the temperature of the system increases, the band gap of perovskite becomes narrow. As a result, the solar cell can no longer absorb photons in the visible range, and the overall efficiency of the system decreases.

***Charge Carrier Mobility*:**When temperature of system rises, mobility of charges in perovskite layer decreases. This is because the thermal energy causes more collisions between the charge carriers, which slow them down. As an outcome, current and efficiency of system drops.

***Crystalline Structure*:**Perovskite solar cells have a polycrystalline structure, which means that they consist of many small crystals. When the temperature of the system increases, these crystals can start to grow and merge, which can lead to defects in the crystal structure. These defects can trap charge carriers, reducing their mobility and overall efficiency.

***Device Stability*:**Perovskite solar cells are known to be unstable at higher temperatures. The thermal stress can cause the device to become less stable, causing a loss of efficiency over time. Therefore, it is important to consider device stability when designing PSCs for extraordinary-temperature applications.

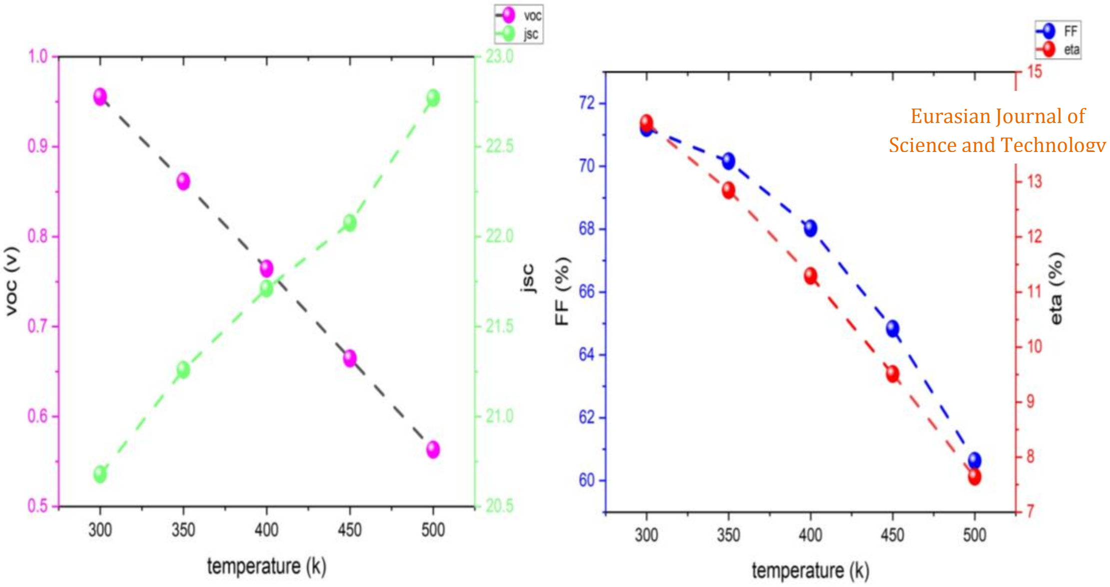

Figure 4 (a) Effect of temperature on Voc and Jsc and (b) Effect of temperature on FF and eta

Conclusion

A lead-free perovskite solar cell was introduced using the non-toxic $FASnI_3$, based on tin (Sn). The study includes a thorough analysis conducted through SCAPS 1D simulation software. The results showed that optimizing the thickness and acceptor density of HTL in ITO/PEDOT:PSS/$FASnI_3$/BCP/Au solar cells can enhance their efficiency, while an increase in temperature adversely affects performance. Through simulation in conjunction with experimental work, the study achieved an important efficiency of 14.07% for the ITO/PEDOT:PSS/$FASnI_3$/BCP/Au solar cell, exhibiting promising characteristics such as Voc (0.95 V), Jsc (20.67 mA/cm^2), and FF (71.21%). This suggests a significant advancement in lead-free perovskite solar cell technology. In addition, the investigation successfully positions the low-cost and non-toxic $FASnI_3$-based perovskite solar cell as a viable contender within the photovoltaic industry.

Acknowledgments

We would like to express our sincere gratitude to all the authors for their immense contribution to this study.

ORCID

Imosobomeh L. Ikhioya

https://orcid.org/0000-0002-5959-4427

References

[1]. Shah S.A.A., Sayyad M.H., Khan K., Guo K., Shen F., Sun J., Tareen A.K., Gong Y., Guo Z., Progress towards high-efficiency and stable tin-based perovskite solar cells, *Energies*, 2020, **13**:5092 [Crossref], [Google Scholar], [Publisher]

[2]. Shukla R., Kumar R.R., Punetha D., Pandey S.K., Design perspective, fabrication, and performance analysis of formamidinium tin halide perovskite solar cell, *IEEE Journal of Photovoltaics*, 2023 [Crossref], [Google Scholar], [Publisher]

[3]. Stranks S.D., Eperon G.E., Grancini G., Menelaou C., Alcocer M.J., Leijtens T., Herz L.M., Petrozza A., Snaith H.J., Electron-hole diffusion lengths exceeding 1 micrometer in an organometal trihalide perovskite absorber. *Science*, 2013, **342**:341 [Crossref], [Google Scholar], [Publisher]

[4]. Kojima A., Teshima K., Shirai Y., Miyasaka T., Organometal halide perovskites as visible-light sensitizers for photovoltaic cells, *Journal of the american chemical society*, 2009, **131**:6050 [Crossref], [Google Scholar], [Publisher]

[5]. Tong J., Song Z., Kim D.H., Chen X., Chen C., Palmstrom A.F., Ndione P.F., Reese M.O., Dunfield S.P., Reid O.G., Liu J., Carrier lifetimes of> 1 μs in Sn-Pb perovskites enable efficient all-perovskite tandem solar cells, *Science*, 2019, **364**:475 [Crossref], [Google Scholar], [Publisher]

[6]. Babayigit A., Ethirajan A., Muller M., Conings B., Toxicity of organometal halide perovskite solar cells, *Nature Materials*, 2016, **15**:247 [Crossref], [Google Scholar], [Publisher]

[7]. Li N., Tao S., Chen Y., Niu X., Onwudinanti C.K., Hu C., Qiu Z., Xu Z., Zheng G., Wang L., Zhang Y., Cation and anion immobilization through chemical bonding enhancement with fluorides for stable halide perovskite solar cells, *Nature Energy*, 2019, **4**:408 [Crossref], [Google Scholar], [Publisher]

[8]. Ke W., Kanatzidis M.G., Prospects for low-toxicity lead-free perovskite solar cells, *Nature communications*, 2019, **10**:965 [Crossref], [Google Scholar], [Publisher]

[9]. Liu C., Tu J., Hu X., Huang Z., Meng X., Yang J., Duan X., Tan L., Li Z., Chen Y., Enhanced hole transportation for inverted tin-based perovskite solar cells with high performance and stability, *Advanced Functional Materials*, 2019, **29**:1808059 [Crossref], [Google Scholar], [Publisher]

[10]. Li C., Song Z., Chen C., Xiao C., Subedi B., Harvey S.P., Shrestha N., Subedi K.K., Chen L., Liu D., Li Y., Low-bandgap mixed tin–lead iodide perovskites with reduced methylammonium for simultaneous enhancement of solar cell

efficiency and stability, *Nature Energy*, 2020, **5**:768 [Crossref], [Google Scholar], [Publisher]

[11]. Kapil G., Hayase S., Tin Halide Perovskite Solar Cells. *Hybrid Perovskite Solar Cells:Characteristics and Operation*, 2021, 373 [Crossref], [Google Scholar], [Publisher]

[12]. Koh T.M., Krishnamoorthy T., Yantara N., Shi C., Leong W.L., Boix P.P., Grimsdale A.C., Mhaisalkar S.G., Mathews N., Formamidinium tin-based perovskite with low E g for photovoltaic applications, *Journal of Materials Chemistry A*, 2015, **3**:14996 [Crossref], [Google Scholar], [Publisher]

[13]. Yu B.B., Chen Z., Zhu Y., Wang Y., Han B., Chen G., Zhang X., Du Z., He Z., Heterogeneous 2D/3D tin-halides perovskite solar cells with certified conversion efficiency breaking 14%, *Advanced Materials*, 2021, **33**:2102055 [Crossref], [Google Scholar], [Publisher]

[14]. Burschka J., Pellet N., Moon S.J., Humphry-Baker R., Gao P., Nazeeruddin M.K., Grätzel M., Sequential deposition as a route to high-performance perovskite-sensitized solar cells, *Nature*, 2013, **499**:316 [Crossref], [Google Scholar], [Publisher]

[15]. Lee S.J., Shin S.S., Kim Y.C., Kim D., Ahn T.K., Noh J.H., Seo J., Seok S.I., Fabrication of efficient formamidinium tin iodide perovskite solar cells through SnF2–pyrazine complex, *Journal of the American Chemical Society*, 2016, **138**:3974 [Crossref], [Google Scholar], [Publisher]

[16]. Abdelaziz S., Zekry A., Shaker A. Abouelatta M., Investigating the performance of formamidinium tin-based perovskite solar cell by SCAPS device simulation, *Optical Materials*, 2020, **101**:109738 [Crossref], [Google Scholar], [Publisher]

[17]. Bati A.S., Zhong Y.L., Burn P.L., Nazeeruddin M.K., Shaw P.E., Batmunkh M., Next-generation applications for integrated perovskite solar cells, *Communications Materials*, 2023, **4**:2 [Crossref], [Google Scholar], [Publisher]

[18]. Bati A.S., Hao M., Macdonald T.J., Batmunkh M., Yamauchi Y., Wang L., Shapter J.G., 1D-2D Synergistic MXene-Nanotubes Hybrids for Efficient Perovskite Solar Cells, *Small*, 2021, **17**:2101925 [Crossref], [Google Scholar], [Publisher]

[19]. Bati A.S., Batmunkh M., Shapter J.G., Emerging 2D layered materials for perovskite solar cells, *Advanced Energy Materials*, 2020, **10**:1902253 [Crossref], [Google Scholar], [Publisher]

[20]. Hossain M.K., Toki G.I., Kuddus A., Rubel M.H.K., Hossain M.M., Bencherif H., Rahman M.F., Islam M.R., Mushtaq M., An extensive study on multiple ETL and HTL layers to design and simulation of high-performance lead-free CsSnCl3-based perovskite solar cells, *Scientific Reports*, 2023, **13**:2521 [Crossref], [Google Scholar], [Publisher]

[21]. Zhu Z., Jiang X., Yu D., Yu N., Ning Z., Mi Q., Smooth and compact FASnI3 films for lead-free perovskite solar cells with over 14% efficiency, *ACS Energy Letters*, 2022, **7**:2079 [Crossref], [Google Scholar], [Publisher]

[22]. Lakhdar N., Hima A., Electron transport material effect on performance of perovskite solar cells based on $CH_3NH_3GeI_3$, *Optical Materials*, 2020, **99**:109517 [Crossref], [Google Scholar], [Publisher]

[23]. Jamal S., Khan A.D., Khan A.D., High performance perovskite solar cell based on efficient materials for electron and hole transport layers, *Optik*, 2020, **218**:164787 [Crossref], [Google Scholar], [Publisher]

[24]. Głowienka D., Zhang D., Di Giacomo F., Najafi M., Veenstra S., Szmytkowski J., Galagan Y., Role of surface recombination in perovskite solar cells at the interface of HTL/$CH_3NH_3PbI_3$, *Nano Energy*, 2020, **67**:104186 [Crossref], [Google Scholar], [Publisher]

[25]. Katariya A., Mahapatra B., Patel P.K., Rani J., Optimization of ETM and HTM layer on NFA based BHJ-organic solar cell for high efficiency

performance, *Optik*, 2021, **245**, 167717. [Crossref], [Google Scholar], [Publisher]

[26]. Saha P., Singh S., Bhattacharya S., Higher efficiency and stability in planar homojunction hybrid antimony (MA3Sb2I9)- based perovskite solar cells, *IEEE Journal of Quantum Electronics*, 2023, **59**:1. [Crossref], [Google Scholar], [Publisher]

[27]. Foster S., Deledalle F., Mitani A., Kimura T., Kim K.B., Okachi T., Kirchartz T., Oguma J., Miyake K., Durrant J.R., Doi S., Electron collection as a limit to polymer:PCBM solar cell efficiency:Effect of blend microstructure on carrier mobility and device performance in PTB7:PCBM, *Advanced Energy Materials*, 2014, **4**:1400311 [Crossref], [Google Scholar], [Publisher]

[28]. Nam W.S., Seo S.H., Park K.H., Hong S.H., Lee G.S., Park J.G., Nonvolatile memory characteristics of small-molecule memory cells with electron-transport and hole-transport bilayers, *Current Applied Physics*, 2010, **10**:37 [Crossref], [Google Scholar], [Publisher]

[29]. Singh N., Agarwal A., Agarwal M., Numerical simulation of highly efficient lead-free all-perovskite tandem solar cell, *Solar Energy*, 2020, **208**:399 [Crossref], [Google Scholar], [Publisher]

[30]. Jayan K.D., Sebastian V., Comprehensive device modelling and performance analysis of MASnI3 based perovskite solar cells with diverse ETM, HTM and back metal contacts, *Solar Energy*, 2021, **217**:40 [Crossref], [Google Scholar], [Publisher]

[31]. Nagaoka H., Ma F., Dequilettes D.W., Vorpahl S.M., Glaz M.S., Colbert A.E., Ziffer M.E., Ginger D.S., Zr incorporation into TiO2 electrodes reduces hysteresis and improves performance in hybrid perovskite solar cells while increasing carrier lifetimes. *The Journal of Physical Chemistry Letters*, 2015, **6**:669 [Crossref], [Google Scholar], [Publisher]

[32]. Jeyakumar R., Bag A., Nekovei R., Radhakrishnan R., Influence of electron transport layer (TiO 2) thickness and its doping density on the performance of CH 3 NH 3 PbI 3-based planar perovskite solar cells, *Journal of Electronic Materials*, 2020, **49**:3533 [Crossref], [Google Scholar], [Publisher]

[33]. Zhang M., Lyu M., Yun J.H., Noori M., Zhou X., Cooling N.A., Wang Q., Yu H., Dastoor P.C., Wang L., Low-temperature processed solar cells with formamidinium tin halide perovskite/fullerene heterojunctions. *Nano Research*, 2016, **9**:1570 [Crossref], [Google Scholar], [Publisher]
