Pak. Sci. Bull. ISSN 2958-6747
Volume 1 issue 2 ,2022

SIMULATION STUDY OF PEROVSKITE SOLAR CELLS: VARIOUS PARAMETERS AND THEIR ANALYSIS BY SCAPS-1D

Anis Naveed[1], *Aroosa Bibi*[1], *Rimsha Bibi*[1], ***Irfan Ahmad***[*]

[1]*Department of Physics, Government Degree College Balakot Mansehra, Khyber Pakhtunkhawa, Pakistan*

irfanahmed@fudan.edu.cn; swateez.scme.nust@gmail.com.

ABSTRACT

Perovskite solar cells have been considered a breakthrough in Photovoltaic's history. Tremendous research has been carried out on perovskite based solar cells in recent past which lead to a rapid boost in performance in relatively short time span. Geometry and Composition are key determinants of performance parameters of a solar cell device. This study investigated the thickness effect of various layers on performance parameters of PV device in Glass/FTO/ SnO_2/$CH_3NH_3PbI_3$/ Spiro-OMeTAD/Au structure. SCAPS-1D (Solar Cell Capacitance Simulator) is used to simulate the device with varying thickness. Findings of this study reveal that thickness of perovskite material and composition of device are key factors in efficiency of the device. Further research in this direction can result in more efficient perovskite based photovoltaic devices.

Keywords: Perovskite solar cells, Simulation study, Photovoltaic, Scaps-1D software,

1. INTRODUCTION

The world today is almost entirely dependent on energy, but traditional sources of energy are not only limited but also a hazard to the environment[1]. Therefore, sustainable and eco-friendly sources of energy are required to overcome this issue. Hydropower, biogas, wind power and solar energy provide about one third of the world's energy needs[2]. The solar power intercepted on earth is thousands times more than our total needs, which is a potential alternative to the sources that can lead to eventual death of ecosystem[3][4]. Solar cells perform the task by converting intercepting photon's energy into electricity (Photovoltaic effect). This was first observed by Edmund Becquerel in 1839[5]. A century later, group of three scientist developed first silicon based solar cell with efficiency of 4%, pursuit for the best continued for a better performance[6].Although PCE of silicon cells was outstanding, but their fabrication costs were too high, so research for the alternatives brought dye-sensitized

(DSSC) and Bulk heterojunction cells (BHJC) [7]. These cells could not stand longer on the central stage due to their low efficiency and instability. Then, came generation of emerging cells which include perovskite solar cells. This was an important milestone because efficiency of PCS rose sharply from 3.8% to ~26% in a decade which their predecessors were not able to achieve in that time span[8]. But they lack stability, so they cannot sustain ambient environment conditions and decompose quickly into their components at elevated temperature. Secondly lead iodide is a poison which harms living organisms[9].An archetypal PCS possesses layer by layer structure, there is an electron transporting layer (ETL) or (ETM) and a hole transporting layer (HTL) or (HTM), where the free electrons and holes get injected into. Usually, the anode and cathode in the perovskite solar cell structure are formed by Fluorine-doped tin oxide (FTO) glass and metal. The Perovskite material is sandwiched between ETM and HTM as in figure 1.

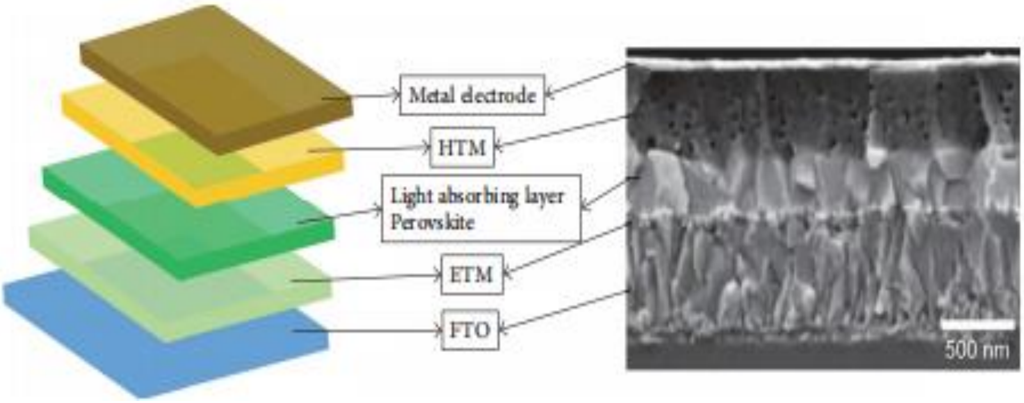


Figure 1: Schematic diagram and SEM image of planar heterojunction structure PSCs.[10]

Their excellent optoelectronic properties like high absorption, low exciton bi long diffusion length, direct tunable bandgap attracted a deal of research[11]. These characteristics arise from their structure and composition which can be altered. Their general formula is ABX_3 where A and B are cations and X is halide anion. For instance, $MAPbI_3$, $FAPbI_3$, $CsPbI_3$ are some well-known compounds, first being the most famous. Hybrid organic-organic perovskites (HOIP) have been proved to most efficient but they lack stability. There have also been studies which suggest that toxic lead could be replaced by Tin (Sn), but efficiency is compromised when this modification is made so there is huge room for development. There are various other parameters such as carrier concentration, bandgap, crystal defects, carrier mobility etc that impact PCE of a working device. The purpose of all structural and compositional changes is to increase stability along with the efficiency so that they can be used commercially, and this will be possible if PCS are resilient to harsh weather[12]. The thickness of the active layer is one of the main parameters affecting PCE of perovskite cell. It needs to be tuned very carefully to maximize the current density and not too large to minimize the reverse saturation current. For devices with thicker active layer most of the harvested light adds to the current but an overly thicken device can cause decline in Fill Factor and V_{OC} which results in low PCE[13].

2. Methodology

This study is aimed at finding thickness effects on performance parameter (V_{oc}, $J_{sc}$and FF) by testing them in SCAPS-1D. SCAPS employs mathematical equations in one dimension to performs its operations.

Some of equations that govern the SCAPS operations are;

$$\frac{d}{dx}\left(-\varepsilon(x)\frac{d\psi}{dx}\right) = q[p(x) - D(x) + N_d^+(x) - N_a^-(x) + p_t(x) - n_t(x)] \ldots\ldots\ldots\ldots (1)$$

is famous Poisson's Equation, while;

$$\frac{dp_n}{dt} = G_p - \frac{p_n - p_{n0}}{\tau_p} - p_n\mu_p\frac{d\xi}{dx} - \mu_p\xi\frac{dp_n}{dx} + D_p\frac{d^2p_n}{dx^2} \ldots\ldots\ldots\ldots (2)$$

$$\frac{dn_p}{dt} = G_n - \frac{n_p - n_{p0}}{\tau_n} + n_p\mu_n\frac{d\xi}{dx} + \mu_n\xi\frac{dn_p}{dx} + D_n\frac{d^2n_p}{dx^2} \ldots\ldots\ldots\ldots (3)$$

are equations of continuity for holes and electrons, respectively. In above mathematical relations $\boldsymbol{\psi}$ is electrostatic potential, $\boldsymbol{D}$ is diffusion coefficient, G is generation rate, $\boldsymbol{\xi}$ is permittivity while $\boldsymbol{n}, \boldsymbol{p}, \boldsymbol{n_t}$ and $\boldsymbol{p_t}$ represent free electrons, free holes, trapped electrons and trapped holes respectively. $\boldsymbol{N_d^+}$ is ionized donor density and $\boldsymbol{N_a^-}$ is ionized acceptor density[].

Performance parameters of a PV device are;

$$V_{OC} = \frac{nKT}{q}\left(ln\frac{I_c}{I_o} + 1\right) \ldots\ldots\ldots\ldots (4)$$

$$J = J_o\left[\exp\left(\frac{qT}{nKT}\right) - 1\right] - J_{sc} \ldots\ldots\ldots\ldots (5)$$

V_{OC}, J_{SC} and J_o are open circuit voltage, short circuit current and saturation current density respectively. Power conversion efficiency (η) is given as below:

$$\eta = \frac{P_{out}}{P_{in}} = \frac{[FF * V_{OC} * J_{sc}]}{P_{in}} \ldots\ldots\ldots\ldots (6)$$

$$FF = \frac{V_{mp}J_{mp}}{V_{OC}J_{sc}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (7)$$

Where V_{mp} and J_{mp} are voltage and current at maximum power point respectively.

Working point condition have been kept as default and thermal effects have not been taken into account, also moisture effects are neglected. Although drastic changes in efficiency occur with change in working temperature as reported by Usha et al[14]

Cell architecture consists of FTO, TiO_2, CH3NH3PbI3, Spiro-OMeTAD and gold contact piled on a transparent glass substrate as shown in figure 2.

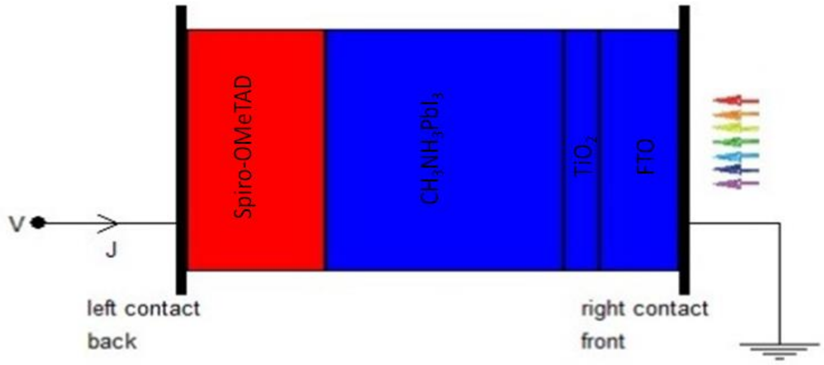


Figure 2: Employed Solar Cell Architecture

The layer parameters used in the simulation are taken from literature [15][16][17][18] and are summarized in (Table 1).The device performance is mainly dependent on electrical, optical and device parameters that are employed in simulation and are given in (Table 2), to achieve realistic results defects in bulk are also introduced. The working points were 0V for bias voltage, 300k for temperature and $1X10^7$ Hz for frequency. Temperature effects were not studied although variation in temperature has significant effects on all the performance parameters.

Table 1: Layer parameters used for simulation Perovskite solar cells.

Parameter associated with solar cell	SnO2:F (FTO)	SnO_2(ETL)	$MAPbI_3$ (Absorber)	Spiro-OMeTAD HTL
Thickness (nm)	$100\ (varied)$	$50\ (varied)$	$600\ varied$	350
Bandgap, E_g (eV)	3.600	3.600	1.500	3.00
Electron affinity χe (eV)	4.000	3.900	3.900	2.100
Relative dielectric permittivity, ε_r	9.000	8.000	30.000	3.000
CB effective density (cm-^{3})	2.200×10^{18}	3.160×10^{18}	2.200×10^{18}	2.200×10^{18}
VB effective density (cm-^{3})	1.800×10^{19}	1.800×10^{19}	1.800×10^{19}	1.800×10^{19}
Thermal velocity of electron (cm/s)	1.00×10^7	1.00×10^7	1.00×10^7	1.00×10^7
Thermal velocity of hole (cm/s)	1.00×10^7	1.00×10^7	1.00×10^7	1.00×10^7
Electron mobility, μ_n (cm2 /Vs)	20	20	2	1.00×10^{-4}
Hole mobility, μ_p (cm2 /Vs)	10	10	2	1.00×10^{-4}
Donor density N_D (cm-^{3})	1×10^{18}	1×10^{18}	1×10^{13}	0
Acceptor density N_A (cm-^{3})	0	0	1×10^{12}	2.00×10^{18}

Table 2: The defect parameters for the Gaussian distribution

Layer	SnO_2:F (FTO)	SnO_2(ETL)	$MAPbI_3$ (Absorber)	Spiro-OMeTAD HTL

Defect type	Neutral	Neutral	Neutral	Neutral
Capture cross section electrons (cm²)	1.00×10^{-15}	1.00×10^{-15}	1.00×10^{-15}	1.00×10^{-15}
Capture cross section holes (cm²)	1.00×10^{-15}	1.00×10^{-15}	1.00×10^{-15}	1.00×10^{-15}
Energetic distribution	Gaussian	Gaussian	Gaussian	Gaussian
Total defect density	1.00×10^{15}	1.00×10^{15}	2.50×10^{13}	1.00×10^{15}

3. RESULTS AND DISCUSSION

3.1. EFFECT OF $MAPBI_3$ THICKNESS

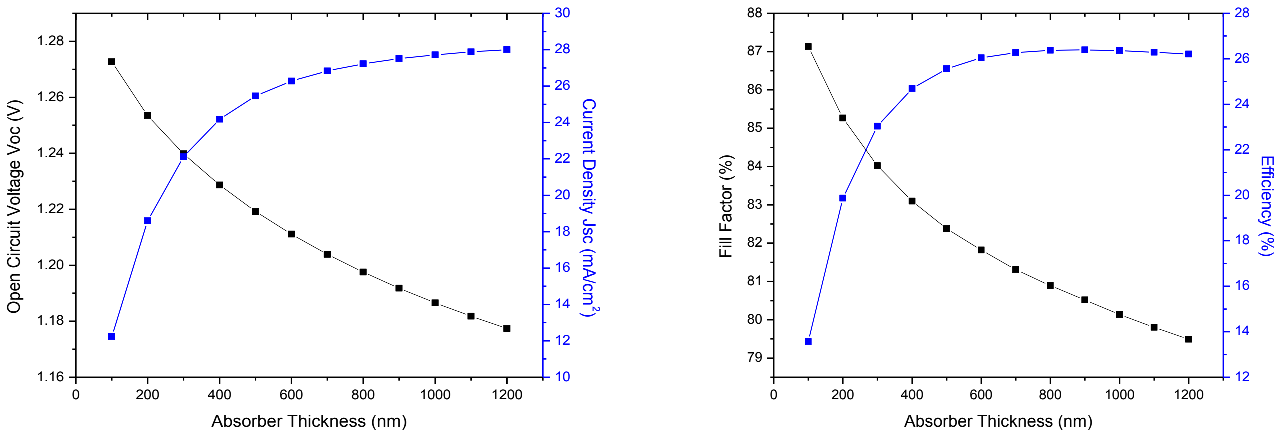
Overall performance of a PV device depends mainly upon photoabsorber layer, so its thickness was varied to study impact on the efficiency of the device. Main layer Thickness was incremented from 100 nm to 1200 and it was observed that current density also increases and then on further increase current becomes constant which is shown in initially rising and then a straight trend in Figures 3.a The density increases from 12 mA/cm^2 to 28 mA/cm^2 . This can be associated with large number of charge carriers produced in a wide layer High absorption of main layer might be an adding factor[19]. Open circuit voltage drops down due to recombination currents when thickness grows larger than diffusion length [20][21].

From Figures 3.b it can be seen that fill factor decreases from 87.5% to 13.5%, as thickness of perovskite layer increases from 100 nm to 1200 nm due to resistive losses. Current density overshadows this decline and in FF and there is a increase in efficiency of device till 850 nm and then it eventually falls due to low recombination and reduced charge carrier extraction. This simulation shows that suitable thickness for absorber layer is around about 850 nm.

3.2. EFFECT OF ETL THICKNESS

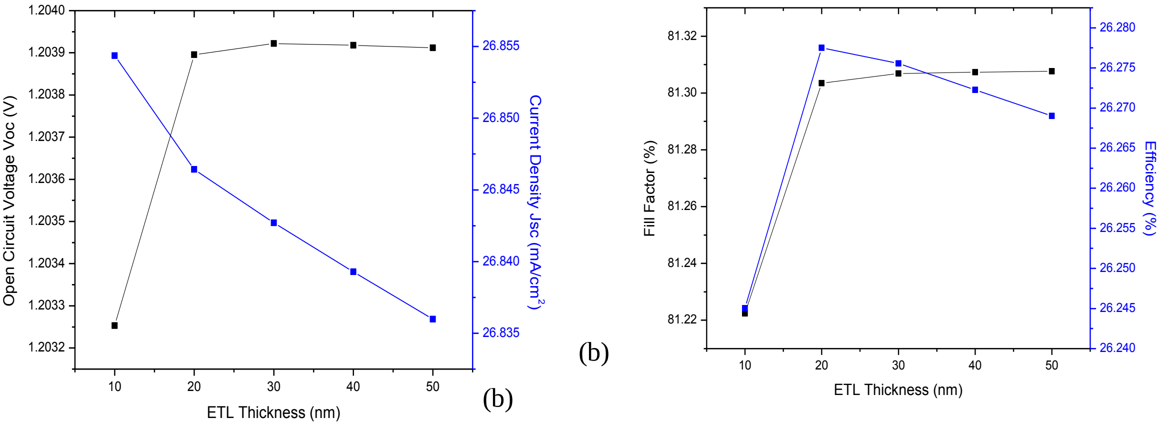
There is a vital role of electron extracting materials in multilayer PV devices. ETM blocks holes and allows electro thus to prevent recombination. In this study its thickness was tuned from 10 nm to 50 nm and influence the variation was other observed. While varying thickness other parameters were kept constant so to investigate the influence of sole thickness variation. Results are given in figures 4. It shows that there is a minute decrease in current density J_{sc} and a little increase in open circuit V_{oc}.

3.3. Effect of FTO thickness: Transparent conducting oxide performs dual task. It acts as front electrode as well as a backside reflector. Its thickness study was also done in order to analyze its impact on performance parameters of the solar cell. Thickness was increased from 10 nm to 450 nm and a minute decline in both the parameters V_{oc} and J_{sc} was observed. J_{sc} fell from 26.84 mA/cm^2 to 26.73 mA/cm^2 while Open circuit voltage reduced to1.20376V from 1.20391V with increase in thickness. This can be attributed to absorption, internal scattering and prolonged paths for carriers. Increased absorption implies less number of photon reaching the photo absorber. Fill factor rises and efficiency falls down due decrease in current and open circuit voltage. Results are given in figures 5.

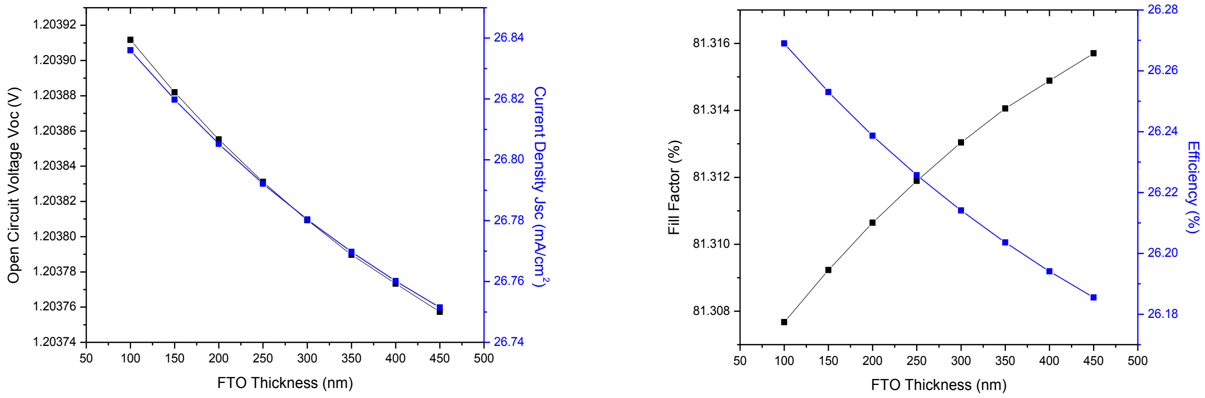


(a) (b)

Figures 3: (a) Open circuit voltage and current density (b) Fill Factor and efficiency as function of $MAPbI_3$ thickness



Figures 4: (a) Open circuit voltage and current density (b) Fill Factor and efficiency as function of SnO_2 thickness



Figures 5: (a) Open circuit voltage and current density (b) Fill Factor and efficiency as function of FTO thickness

4. CONCLUSION

Perovskite solar cell was simulated and analyzed in this study with (n-i-p) architecture Spiro-OMeTAD/$MAPbI_3$/SnO_2/FTP .Thickness of each layer was varied to study their influence on performance parameters of the cell. It was observed that thickness of main layer is greater and 800 nm to 900 nm thick layers are suitable for high efficiency. Further it was revealed that variation in ETL has not significant on device performance. Thickness of 100 nm is suitable, greater thickness can lead to lowered efficiency. This Study has determined the key role of geometry and composition perovskite based solar cell devices. Further Studies on compositional engineering and geometrical variations can result in more efficient devices.

5. Acknowledgments

Mr.Burgleman deserves our sincere thanks for he allowed us to use SCAPS-1D which is developed by him and his colleagues at university. This article would not have accomplished if Dr Irfan Ahmad were not there to guide and support us .We are also deeply grateful to him.

6. REFERENCES

[1] N. L. Panwar, S. C. Kaushik, and S. Kothari, "Role of renewable energy sources in environmental protection: A review," *Renew. Sustain. Energy Rev.*, vol. 15, no. 3, pp. 1513–1524, 2011, doi: 10.1016/j.rser.2010.11.037.

[2] N. Armaroli and V. Balzani, "Solar Electricity and Solar Fuels: Status and Perspectives in the Context of the Energy Transition," *Chem. – A Eur. J.*, vol. 22, no. 1, pp. 32–57, Jan. 2016, doi: https://doi.org/10.1002/chem.201503580.

[3] R. T. Oğulata and S. N. Oğulata, "Solar Energy Potential in Turkey," *Energy Sources*, vol. 24, no. 12, pp. 1055–1064, Dec. 2002, doi: 10.1080/00908310290086987.

[4] F. Barbir, T. N. Veziroğlu, and H. J. Plass Jr, "Environmental damage due to fossil fuels use," *Int. J. Hydrogen Energy*, vol. 15, no. 10, pp. 739–749, 1990.

[5] H. Zou *et al.*, "Alternating current photovoltaic effect," *Adv. Mater.*, vol. 32, no. 11, p. 1907249, 2020.

[6] D. Schultz and L.-C. Campeau, "Harder, better, faster," *Nat. Chem.*, vol. 12, no. 8, pp. 661–664, 2020.

[7] F. F. Targhi, Y. S. Jalili, and F. Kanjouri, "MAPbI3 and FAPbI3 perovskites as solar cells: Case study on structural, electrical and optical properties," *Results Phys.*, vol. 10, pp. 616–627, 2018, doi: 10.1016/j.rinp.2018.07.007.

[8] L. Lin *et al.*, "Inorganic electron transport materials in perovskite solar cells," *Adv. Funct. Mater.*, vol. 31, no. 5, p. 2008300, 2021.

[9] W. Ke and M. G. Kanatzidis, "Prospects for low-toxicity lead-free perovskite solar cells," *Nat. Commun.*, vol. 10, no. 1, pp. 1–4, 2019.

[10] D. Zhou, T. Zhou, Y. Tian, X. Zhu, and Y. Tu, "Perovskite-Based Solar Cells: Materials, Methods, and Future Perspectives," *J. Nanomater.*, vol. 2018, p. 8148072, 2018, doi: 10.1155/2018/8148072.

[11] S. A. Olaleru, J. K. Kirui, D. Wamwangi, K. T. Roro, and B. Mwakikunga, "Perovskite solar cells: The new epoch in photovoltaics," *Sol. Energy*, vol. 196, pp. 295–309, 2020, doi: https://doi.org/10.1016/j.solener.2019.12.025.

[12] L. Qiu, L. K. Ono, and Y. Qi, "Advances and challenges to the commercialization of organic–inorganic halide perovskite solar cell technology," *Mater. today energy*, vol.

7, pp. 169–189, 2018.

[13] M. Rai, L. H. Wong, and L. Etgar, “Effect of Perovskite Thickness on Electroluminescence and Solar Cell Conversion Efficiency,” *J. Phys. Chem. Lett.*, vol. 11, no. 19, pp. 8189–8194, Oct. 2020, doi: 10.1021/acs.jpclett.0c02363.

[14] U. Mandadapu, S. V. Vedanayakam, and K. Thyagarajan, “Numerical simulation of Ch3Nh3PbI3-XClx perovskite solar cell using SCAPS-1D,” *Int J Eng Sci Invent.*, vol. 2, pp. 40–45, 2017.

[15] W. Isoe, M. Mageto, C. Maghanga, M. Mwamburi, V. Odari, and C. Awino, “Thickness dependence of window layer on CH3NH3PbI3-XClX Perovskite solar cell,” *Int. J. Photoenergy*, vol. 2020, 2020.

[16] H. Sabbah, “Numerical Simulation of 30% Efficient Lead-Free Perovskite CsSnGeI3-Based Solar Cells,” *Materials (Basel).*, vol. 15, no. 9, p. 3229, 2022.

[17] F. Anwar, R. Mahbub, S. S. Satter, and S. M. Ullah, “Effect of different HTM layers and electrical parameters on ZnO nanorod-based lead-free perovskite solar cell for high-efficiency performance,” *Int. J. Photoenergy*, vol. 2017, 2017.

[18] N. Shukla, D. Prajapati, and S. Tiwari, “Investigation on Design and Device Modeling of High Performance CH3NH3PbI3-xClx Perovskite Solar Cells,” *J. Ravishankar Univ.*, vol. 34, no. 1, pp. 58–63, 2021.

[19] Z. Lian *et al.*, “High-performance planar-type photodetector on (100) facet of MAPbI3 single crystal,” *Sci. Rep.*, vol. 5, no. 1, pp. 1–10, 2015.

[20] A. Bag, R. Radhakrishnan, R. Nekovei, and R. Jeyakumar, “Effect of absorber layer, hole transport layer thicknesses, and its doping density on the performance of perovskite solar cells by device simulation,” *Sol. Energy*, vol. 196, pp. 177–182, 2020.

[21] L. M. Pazos-Outón, T. P. Xiao, and E. Yablonovitch, “Fundamental efficiency limit of lead iodide perovskite solar cells,” *J. Phys. Chem. Lett.*, vol. 9, no. 7, pp. 1703–1711, 2018.