Recent Progress in the Development of High-Efficiency Perovskite Solar Cell Using Copper Iodide (CuI) as Hole Transport Layer

Abstract— *Solar cells are a practical option that could potentially require additional energy sources for developing new clean energy. A renewable source of electricity is characterized by its affordability, accessibility, and zero emissions from greenhouse gases. By converting sunlight photons into electrical power, photovoltaic cells are a viable option. The last two decades have witnessed numerous material opportunities for scientific advancements in photovoltaic technology, which have resulted in reduced costs and improved solar cell efficiency. Perovskite materials represent a captivating class of compounds distinguished by their diverse applications, particularly in the realm of solar energy. Renowned for their distinct crystal structure and versatile characteristics, perovskites possess a myriad of noteworthy parameters and properties. The hole transport layer (HTL) plays important role in the efficacy of solar cells using perovskite material such as CH3NH3PbI3 with solar cell simulator software (SCAPS) Tool. The Quantitative simulation and modeling have been used to determine the electrical characteristics of the MAPbI3 material used for the active layer for a few parameters, including fill factor (FF), short-circuit current density (Jsc), power conversion rate (PCE), and open-circuit voltage (Voc). Calculations have been made for the capacitance-frequency (C-F) and capacitance-voltage (C-V) of the previously studied perovskite solar cell. The simulated findings demonstrate that the MAPbI3 has specifications for performance such as FF=86.59, PCE=29.54, Voc=1.1837, and Jsc=28.82 mAcm^{-2}. Copper Iodide (CuI) material plays a crucial role as a hole transmitting Layer (HTL).*

Keyword—Perovskite solar cell, $CH_3NH_3PbI_3$, CuI, C-f, C-V, FF, V_{oc}, J_{sc}, and PCE

I. INTRODUCTION

Solar cells are a practical option that could potentially require additional energy sources for developing new clean energy. A renewable source of electricity is characterized by its affordability, accessibility, and zero emissions from greenhouse gases[1]. By converting sunlight photons into electrical power, photovoltaic cells are a viable option. The last two decades have witnessed numerous material opportunities for scientific advancements in photovoltaic technology, which have resulted in reduced costs and improved solar cell efficiency. In 1954, Bell Laboratories developed the first efficient photovoltaic system, which achieved 6%[3]. Silicon solar panels with a 1. Single cell "photovoltaic" devices are often more efficient with a 1 eV band gap. The low weight and flexibility of lightweight film solar cells are additional advantages. The use of materials such as organic dye, conductive polymers, and silicon wire is common in third-generation solar cells, which also employ larger band gaps. The development of photovoltaic cells is the expected to be a crucial step in the progress of renewable energy sources in near future. They are an infinite supply and can be obtained without emitting carbon dioxide[2-9]. Sustainable energy can be produced using only the sun, tides, wind, and rain as natural resources. Solar energy is both safe and beneficial for our health, in our homes and Businesses[10-15]. In the future, solar cells may be the primary source of renewable energy. The most dependable and stable form of free energy is now solar power. A multitude of other elements within the perovskite family could make a significant impact. CuI's chemical stability, easy synthesis, and high transparency in the visible spectrum are among its other significant advantages. Even though CuI is processed in DES solvents, the perovskite layer may undergo degradation. As a result, researchers attempted to create CuI-based PSCs through p-in arrangements[17].. Ye et al.[26] A film of CH3NH3PbI3 with X=I, Br, and Cl was rapidly deposition-crystallized after a layer of CuI was electrodeposited in 2015. The mean PCE was 15. A remarkable PCE of 16 and a score of 6%. CuI-founded PSCs attained a 6% success rate, which could be linked to the exceptionally high hole mobility for Cu(H)CN HTL. The small interface resistance to contact and low apparent coarseness of the resulting perovskite films allowed for this. In addition, it has been shown that special, unconventional methods are used to create the perovskite layer. The effectiveness of the holes transport layer (HTL) of $CH3NH3PbI_3$, X=I solar cells made from perovskite and inorganic copper iodide (CuI), is investigated[16-23].

A solar cell, also referred to as a photovoltaic cell, functions by directly converting sunlight into electricity through a process known as the photovoltaic effect. Below is a simplified overview of how a solar cell operates:

1. **Sunlight Absorption:** Solar cells are typically crafted from semiconductor materials like silicon. When sunlight, comprised of photons, strikes the solar cell's surface, a portion of these photons is absorbed by the semiconductor material.

2. **Creation of Electron-Hole Pairs:** Upon absorption, photons transfer their energy to electrons within the semiconductor, elevating them to higher energy states. This generates electron-hole pairs, where electrons gain freedom to move, leaving behind positively charged "holes" in the material.

3. **Charge Carrier Separation:** The internal electric field within the semiconductor material prompts the free electrons and positively charged holes to move in opposite directions, thus separating the charge carriers.

4. **Charge Carrier Collection:** Metal contacts positioned on the top and bottom surfaces of the solar cell facilitate the collection of separated electrons and holes. These contacts enable the flow of electrons (current) out of the cell for external electrical applications[22].

5. **Conversion of Light Energy to Electrical Energy:** When an external circuit is connected to the solar cell, the movement of electrons through the circuit generates an electric current. This current can power electrical devices or be stored in batteries for later use[21].

6. **Operation in Closed Circuit:** As long as sunlight is available and the circuit remains closed, the flow of electrons through the external circuit persists. However, when the circuit is opened or sunlight is obstructed, the flow of electrons halts.

In essence, a solar cell utilizes sunlight's energy to produce an electric current, offering a renewable and sustainable source of electricity. Multiple solar cells can be interconnected to form solar panels, enhancing the electricity generation capacity for residential, commercial, or industrial applications[20].

2. PEROVSKITE MATERIAL

Perovskite materials represent a captivating class of compounds distinguished by their diverse applications, particularly in the realm of solar energy. Renowned for their distinct crystal structure and versatile characteristics, perovskites possess a myriad of noteworthy parameters and properties.

Crystallographic ally, perovskites adopt a general formula denoted as ABX_3, wherein the cations 'A' and 'B' vary in size (with 'A' typically larger than 'B'), while 'X' signifies an anion. Their crystalline arrangement can manifest in cubic, tetragonal, or orthorhombic structures, contingent upon environmental conditions.

Their optical absorption capabilities are noteworthy, demonstrating substantial absorption and a modifiable band gap, crucial attributes underpinning their efficacy in photovoltaic applications. Perovskites excel in charge transport, showcasing extended diffusion lengths, ambipolar charge mobility, and elevated carrier mobility, all pivotal for efficient energy conversion. Furthermore, their robust tolerance to point defects contributes to enhanced stability and performance, a trait highly advantageous in various applications[23].

Certain perovskite variants, particularly those incorporating cobalt, exhibit magnetic properties attributable to cobalt's inherent spin. Additionally, through doping—a process involving the introduction of impurities—perovskite properties, both optical and electrical, can be finely tuned to suit specific requirements[25].

These materials are broadly classified into two categories: purely inorganic perovskites, exemplified by compounds like $PbTiO_3$ and $CaSiO_3$, and organic-inorganic hybrid perovskites, typified by compositions such as $CH_3NH_3MX_3$ (where M = Pb or Sn; (X = I).

3. ADVANTAGES OF PEROVSKITE MATERIALS:

1. High Efficiency: Perovskite solar cells offer competitive efficiency, promising cost-effective solar energy generation.

2. Tenable Properties: Their customizable band-gap allows for tailored optical and electronic characteristics, enhancing versatility in various applications.

3. Abundance and Low-Cost Production: Composed of abundant and inexpensive elements, perovskite materials hold promise for scalable, cost-effective manufacturing methods.

4. Versatility: Perovskite materials find application beyond solar cells, including LEDs, sensors, and photo detectors, due to their diverse forms and properties[21].

4. DISADVANTAGES OF PEROVSKITE MATERIALS:

1. Stability Concerns: Prone to degradation when exposed to moisture, oxygen, and light, limiting long-term reliability, and commercial viability[22].

2. Toxicity Issues: Some formulations contain lead, raising environmental and health concerns during manufacturing, usage, and disposal.

3. Scaling Challenges: Challenges in maintaining consistent quality and efficiency during large-scale production hinder commercial adoption[23].

4. Material Reproducibility: Achieving reproducible performance across different batches remains a challenge due to variations in synthesis techniques and processing conditions.

5. FUTURE SCOPE OF PEROVSKITE MATERIALS:

1. Commercialization of Perovskite Solar Cells: Research focuses on enhancing stability and scalability for widespread adoption in solar energy production.

2. Exploration of Lead-Free Alternatives: Development efforts aim to develop eco-friendly formulations to address toxicity concerns and broaden market acceptance.

3. Diversification into Emerging Technologies: Perovskite materials are being investigated for applications beyond photovoltaics, including LEDs, sensors, and optoelectronic devices.

4. Integration with Existing Infrastructure: Efforts concentrate on seamlessly integrating perovskite technologies with established semiconductor platforms to leverage synergies and enhance performance.

6. APPLICATIONS OF PEROVSKITE MATERIALS:

1. Solar Energy: Perovskite solar cells are used to generate electricity from sunlight, offering a promising alternative to traditional silicon-based solar cells15].

2. LEDs and Lighting: Perovskite materials show potential for efficient and tenable light emission, making them suitable for LED technologies[20].

3. Sensors and Photo detectors: Perovskite-based sensors and photo detectors offer high sensitivity and response, enabling applications in environmental monitoring, biomedical devices, and security systems[7].

4.Optoelectronic Devices: Perovskite materials are utilized in various optoelectronic devices, including lasers, displays, and detectors, due to their excellent optical and electronic properties

7. FABRICATION OF PEROVSKITE SOLAR CELL

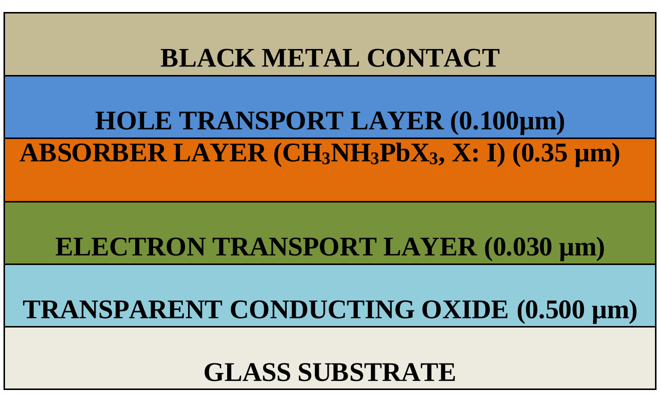

Fig 1 Fabrication of Solar Cell Using Perovskite Material

The "planer heterogeneous junction" structure and perovskite photovoltaic cells (PSCs) have identical configurations. The transport electron layer comprises silicon dioxide (TiO_2), while the glass substratum layer is made of transport conducting oxides (TCO). In perovskite materials, CuI serves as the hole transport layer (HTL) for the metal reverse contact, while $CH_3NH_3PbI_3$, X=I, serves as the active layer. Fabrication of Solar Cell Using Perovskite Material is shown in Figure 1.

The photovoltaic effect, generating electricity from sunlight without emitting gases like carbon dioxide or other pollutants such as sulfur or nitrogen, is fundamental to photovoltaic cells. Solar cells can also indirectly convert solar energy into electricity by first converting it into heat or other forms of chemical energy, without posing risks to the environment or human health. Solar cells are a low-maintenance, durable energy source that can be easily installed in various locations, including homes, workplaces, caravans, tourist attractions, calculators, watches, light meters, and cameras. Solar cells offer an affordable, efficient, and environmentally friendly power source that is non-polluting, non-infectious, and noiseless.

Nowadays, global warming poses a serious threat to humankind and the stability of wildlife on Earth. Sea levels have risen by 10–25 cm, and surface temperatures have increased by 0.3–0.6 during the 19th century due to global warming. Rising sea levels have led to increasingly severe natural disasters and disruptive impacts on human life and other living processes across the planet in the coming years.

Solar panels are set up with an enormous array of tiny cells to generate a specific amount of power. The goal of current solar cell technologies is to create electrons and holes in each cell. CuI acts as the HTL for the metal back contact, and CH3NH3PbI3 from the piezoelectric family makes up the active layer. CuI material serves as the HTL in perovskite solar cells, enhancing the cell's efficiency. Studies indicate that spiro-MeOTAD has a larger fill factor (FF) and lower electrical conductivity than CuI. The exceptional power conversion efficiency (PCE) of 16.6% achieved by CuI-based PSCs, exceeding the median PCE of 15.6%, could potentially be attributed to the high hole mobility of the CuI HTL. The minimal surface roughness and low interface resistance to contact of the resulting perovskite films allowed for this. Additionally, specifically designed methods have been shown to effectively reduce the degradation of the perovskite layer caused by the synthesis of CuI in the n-i-p PSC solution, where the active layer is represented by $CH_3NH_3PbI_3$, X=I.

8. PARAMETERS OF A SOLAR CELL

1. Efficiency: This determines the quantity of sunlight that is turned into useful power. It's one of the most crucial elements since higher efficiency means that for a given amount of sunlight, more power is produced.

2. Open-Circuit Voltage (Voc): When a solar cell is not connected to any load, its maximum voltage can be produced.

When the solar cell is not receiving any current, that voltage is present.

3. Short-Circuit Current (Isc): The maximum current that a solar cell can generate when its electrical connections are made short. Voltage between the solar cell is absent when the current is zero.

4. Fill Factor (FF): This number represents the photovoltaic cell's theoretical closest point to delivering its maximum power output. It is calculated by dividing the total power of the solar cell by the product of its open-circuit voltage, short-circuit current, and voltage and current at the maximum power point.

5. Maximum Power Point (Pmax): the point on the current-voltage (I-V) curve of a solar cell when the product of current and voltage is at its maximum. It displays the maximum power that the solar cell can produce in a given situation.

6. Temperature Coefficient: This metric indicates how temperature variations affect the solar cell's performance. Generally, efficiency drops with increasing temperature.

7. Shunt Resistance (Rsh): The resistance measured in this manner is parallel to the p-n junction of the solar cell. It is an illustration of the solar cell's leakage current route.

8. Series Resistance (Rs): This resistance is determined by measuring it in series with the p-n junction of the solar cell. It takes into consideration the resistive losses in the solar cell.

9. RESULTS AND DISCUSSION

Table II provides the many performance metrics for the perovskite cell CH3NH3PbX3 (X: I), including Jsc, FF, Voc, C-F, C-V, and PCE. The effectiveness of the cell has been established. There are two illumination settings used for the simulation: low and high. When utilizing CuI as a hole transport layer, the results are different from what other searchers have reported. The working point voltages under both dark and light circumstances are zero and 0.5V, respectively, for all of the perovskite solar cell materials that have been studied. The different determined features for the investigated perovskite solar cell are listed in Table II.

TABLE.II The variously computed characteristics of the perovskite solar cell under study (CH3NH3PbX3, X: I)

MATERIAL		PARAMETER			
		V_{oc}(V)	J_{sc}(mAcm^{-2})	FF	PCE (%)
$CH_3NH_3PbI_3$	Present Work	1.1837	28.825884	86.59	29.54

Comparing the CH3NH3PbI3 perovskite solar cell to those of other researchers, the simulated findings show parameters for performance such Voc=1.183, Jsc=28.82, FF=89.59, and PCE=29.54 .
Regarding the examined perovskite solar cell, figure 2 provides the specifications of the cell, and the J-V properties have been displayed.

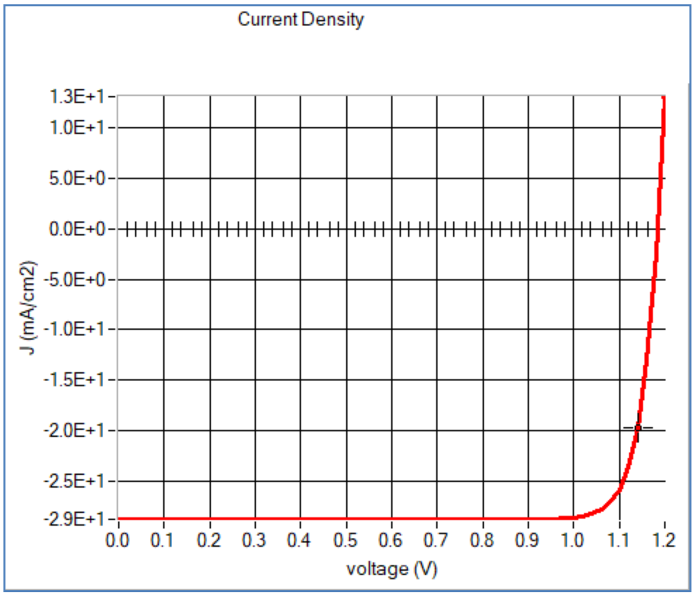

Fig.2.The J-V characteristics for the $CH_3NH_3PbI_3$ perovskite solar cell

For the $CH_3NH_3PbX_3$ (X: I) perovskite solar cell, the current density (JV) characteristics were calculated as seen in Figure2.

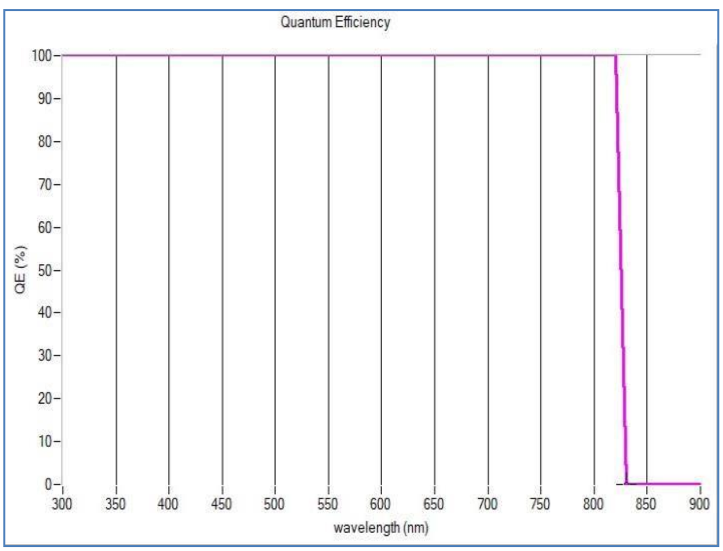

Fig.3. Quantum efficiency of $CH_3NH_3PbI_3$ perovskite solar cell

For the $CH_3NH_3PbX_3$ (X: I) perovskite solar cell, the quantum effectiveness (QE) characteristics were calculated and plotted for an absorption coefficient of 10^7 (cm^{-1}) , as seen in Figure3.

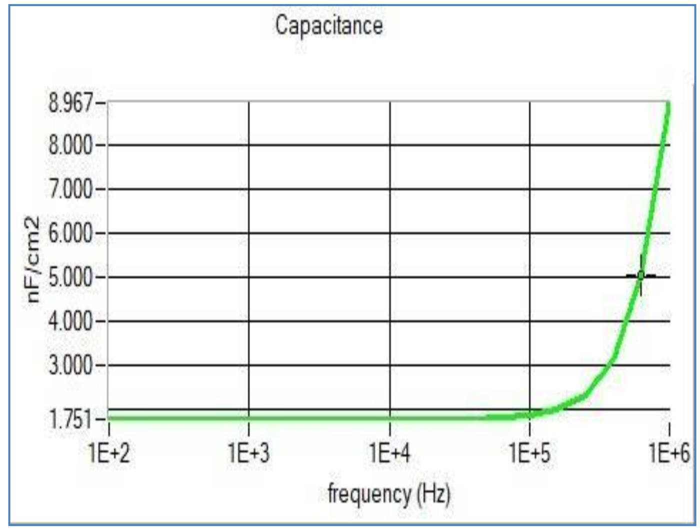

Fig.4. C-f characteristics for$CH_3NH_3PbI_3$ perovskite solar cell

For the $CH_3NH_3PbI_3$ perovskite solar cell under study, the capacitance-frequency (C-f) properties have been determined and are displayed in Figure.4. By adjusting the alternating current signal frequency during the C-f measurements, capacitance is computed. This demonstrates that $CH_3NH_3PbI_3$ is more responsive to capacitance production at higher frequency ranges.

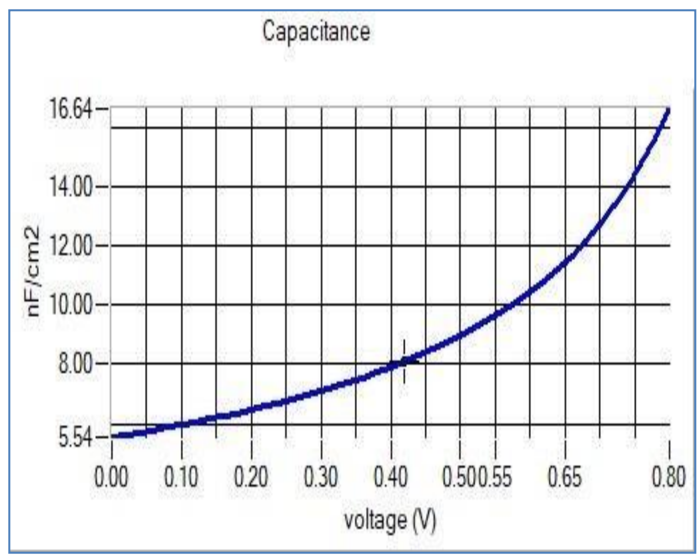

Fig.5.The C-V characteristics of $CH_3NH_3PbI_3$ perovskite solar cell

For a $CH_3NH_3PbI_3$ based solar cell, the variation in capacitance ($nFcm^{-2}$) is measured with regard to the applied voltage, and it increases exponentially with respect to voltage. For $CH_3NH_3PbI_3$, the capacitance ($nFcm^{-2}$) rises and becomes saturated. Figure 5. plots the calculated capacitance (C) vs voltage (V) for the perovskite solar cell under investigation.

CONCLUSION

In the research, The hole transport layer (HTL) play important role in the efficacy of solar cells using perovskite material such as $CH_3NH_3PbI_3$ with solar cell simulator software (SCAPS) Tool. The Quantitative simulation and modeling have been used to determine the electrical characteristics of the MAPbI3 material used for the active layer for a number of parameters, including fill factor (FF), short-circuit current density (Jsc), power conversion rate (PCE), and open-circuit voltage (Voc). Calculations have been made for the capacitance-frequency (C-F) and capacitance-voltage (C-V) of the previously studied perovskite solar cell. The simulated findings demonstrate that the MAPbI3 has specifications for performance such as FF=86.59, PCE=29.98, Voc=1.1837, and Jsc=28.82 mAcm-2. Copper Iodide (CuI) material plays a crucial role as a hole transmitting Layer (HTL)..

REFRENCES

1 M. Hosenuzzaman , N.A. Rahim , J. Selvaraj , M. Hasanuzzaman , A.B.M.A. Malek , A. Nahar, “Global prospects, progress, policies, and environmental impact of solar photovoltaic power generation,” Renewable and Sustainable Energy Reviews 41, 284–297, (2015).

2 Kiran ranabhat, Leev patrikeev, Kirill andrianov, Valerii lapshinsky, Elena sofronova “An Introduction to Solar Cell Technology,” 14(2016)4, 405, 481 - 491.

3 C.-W. Chen, S.-Y. Hsiao, C.-Y. Chen, H.-W. Kang, Z.-Y. Huang and H.-W. Lin, “Optical properties of Organometal halide perovskite thin films and general device structure design rules for perovskite single and tandem solar cells,” 3, 9152-9159, 2015.

4 Giordano F, Abate A, Correa Baena J P, Saliba M, Matsui T,Im S H, Zakeeruddin S M, Nazeeruddin M K,Hagfeldt A and Graetzel M, “Enhanced electronic properties in mesoporous TiO_2 via lithium doping for high efficiency perovskite solar cells,” 7 10379, 2016.

5 M. J. Taghavi, M. Houshmand, M. H. Zandi and N. E. Gorji, “Modeling of optical losses in perovskite solar cells,” 97, 424-428, 2016.

6 Tanuj Tiwari, 2018. “Next generation Soler Power technology”, www.electronicsforu.com, May18,

7 Rashmi Swami, 2012. “Solar Cell,” International Journal of Scientific and Research Publications, Volume 2, Issue 7, July 1 ISSN 2250-3153

8 Mohammad Tawheed Kibria, Akil Ahammed, Saad Mahmud Sony, Faisal Hossain, Shams-Ul-Islam, “A Review Comparative studies on different generation solar cells technology,” ICEAB, Paper ID E33, 2014.

9 Shruti Sharma, Kamlesh Kumar Jain, Ashutosh Sharma, “Solar cell: In Research and Application –A Review Materials Sciences and Applications,” 2015, 6, 1145-1155

10 Dazheng Chen and Chunfu Zhang, “Interface Engineering and Electrode Engineering for Organic Solar Cells”,2016, DOI: 10.5772/65312

11 R. Pandey and R. Chaujar,“Numerical simulations: Toward the design of 27.6% efficient four-terminal semi-transparent perovskite/SiC passivated rear contact silicon tandem solar cell,” 2016,100, 656-666.

12 Z.-L. Huang, C.-M. Chen, Z.-K. Lin and S.-H. Yang,” Efficiency enhancement of regular-type perovskite solar cells based on Al-doped ZnO nanorods as electron transporting layers,” 2017,102, 94-102.

13 W. S. Yang, J. H. Noh, N. J. Jeon, Y. C. Kim, S. Ryu, J. Seo and S. I. Seok, “High-performance photovoltaic perovskite layers fabricated through intra molecular exchange,” Science 348, 1234, 2015.

14 Yu Miyazawa, Masashi Ikegami, Hsin-Wei Chen, Takeshi Ohshima, Mitsuru Imaizumi, Kazuyuki Hirose, Tsutomu Miyasaka, “Tolerance of Perovskite Solar Cell to High-Energy Particle Irradiations in Space Environment,” April 27, Miyazawa et al., iScience 2, 148–155, 2018.

15 J.-P. Correa-Baena, A. Abate, M. Saliba, W. Tress, T. J. Jacobsson, M. Grätzel and A. Hagfeldt, “The rapid evolution of highly efficient perovskite solar cells,” Energy Environ. Sci. DOI: 10.1039/C6EE03397K, 2017.

16 Nandi Wu, Yiliang Wu, Daniel Walter, Heping Shen, The Duong, Dale Grant, Chog Barugkin, Xiao Fu, Jun Peng, Thomas White, Kylie Catchpole, and Klaus Weber. “Identifying the Cause of Voltage and Fill Factor Losses in Perovskite Solar Cells by Using Luminescence Measurements,” DOI: 10.1002 /ente201700374.

17 Syed Zulqarnain Haider, Hafeez Anwar, Mingqing Wang, “A comprehensive device modeling of Perovskite solar cell with inorganic copper iodide as hole transport material,” Semicond. Sci. Technol. 33, 0 35001 (12pp), 2018.

18 J. Verschraegen and M. Burgelman, “Numerical modeling of intra-band tunneling for hetero junction solar cells in SCAPS”, Thin Solid Films, 515 (15), 6276-6279 (2007)

19 Prasanth kumar and Giri babu, 2016. “Recent advances in perovskite-based solar cells”. Curr. Sci., 111 1173–81

20 K. masuko, M. shigematsu, T. hashiguchi, D. fujishima, M. kai, N. yoshimura, T. yamaguchi, Y. ychihashi, T. Yamanishi, T. Takahama, M. Taguchi, E. Maruyama, S. Okamoto, T. Mishima, N. Matsubara, T. Yamanishi, T. Takahama, M. Taguchi, E. Maruyama, and S. Okamoto, “Achievement of More Than 25% Conversion Efficiency with Crystalline Silicon Heterojunction Solar Cell,” IEEE Journal of Photovoltaic Vol.4, Issue6, pp. 1433–1435, 2016.

21 C. Wehrenfennig, G.E. Eperon, M.B. Johnston, H.J. Snaith, L.M. Herz, 2014. “High Charge Carrier Mobilities and Lifetimes in Organolead Tri halide Perovskite”. Journal of Advanced Materials, Vol. 26 , pp. 1584-1589
22 Bottaro and Moscowitz, “Current photovoltaic technology: current progress and future prospects,” 1997, MIT-EL77-041W
23 Homes CC, 2001. “Optical response of high dielectric-constant perovskite related oxide”. science 293 673-6
24 Farzad Sadeghi, Mina Neghabi, “Optimization of structure of solar cells based on lead based perovskite via numerical simulation,” Journal of Solar Energy Research 24, 315- 321, 2017.
25 Jeng J-Y, Chiang Y-F, Lee M-H, Pemg S-R, Guo T-F, Chen P and Wen T-C, “$CH_3NH_3PbI_3$ perovskite/ fullerence planer-hetero junction hybrid solar cells,” 2013, Adv.Mater.25 3727-32
26 Ye Z, Yin X, Chen L, He X, Lin Z, Liu C, Ning S, Wang X, Wei Y. An integrated process for removal and recovery of Cr (VI) from electroplating wastewater by ion exchange and reduction–precipitation based on a silica-supported pyridine resin. Journal of Cleaner Production. 2019 Nov 1;236:117631.

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