

Study of Perovskite ($\text{CH}_3\text{NH}_3\text{PbI}_3$) Solar Cell Using CuI (Copper Iodide) as Hole Transport Layer (HTL) at Different Thickness of HTL Layer

Hemant Kumar Rao^{1*}, Akash Chauhan¹, Md. Asfahan¹, Deepak Gautam¹, Ravi Shankar Yadav², Anchal Yadav²

Abstract

While solar energy is a viable option, future clean energy solutions may require other energy sources. Renewable electricity sources are known for being affordable, easy to access, and not producing greenhouse gases. Photovoltaic cells, which turn sunlight into electrical power, are a good choice. Over the last 20 years, advancements in photovoltaic technology have lowered costs and improved the efficiency of solar cells. Perovskite materials, recognized for their unique crystal structure and flexible properties, are particularly promising for solar energy. The solar cell simulation software (SCAPS) Tool demonstrates that the hole transport layer (HTL) is essential for the efficiency of solar cells employing perovskite materials like $\text{CH}_3\text{NH}_3\text{PbI}_3$. The electrical characteristics of MAPbI_3 material in the active layer have been ascertained using quantitative computations and mathematical models, with particular attention to variables such as fill factor (FF), power conversion efficiency (PCE), short-circuit current density (J_{sc}), and open-circuit voltage (V_{oc}). The capacitance-frequency (C-F) and capacitance-voltage (C-V) of previously researched solar power cells made from perovskite have been calculated. The simulation results show that MAPbI_3 at different thickness of HTL provide FF=86.59, PCE=29.54 watts, V_{oc} =1.1837 V, and J_{sc} =28.82 mA/cm² at the 0.100 thickness and FF=85.64, PCE=29.22 watts, V_{oc} =1.1837 V, and J_{sc} =28.82 mA/cm² at 0.200 thickness and also FF=74.96, PCE=28.97 watts, V_{oc} =1.3408 V, and J_{sc} =28.82 mA/cm² at 0.300 thickness.

Keywords: Perovskite solar cell, $\text{CH}_3\text{NH}_3\text{PbI}_3$, CuI, C-f, C-V, FF, V_{oc} , J_{sc} , PCE

INTRODUCTION

While solar cells are a viable option, the development of new clean energy technologies may

*Author for Correspondence

Hemant Kumar Rao

E-mail: hemant.86019@gmail.com

¹Student, Department of Electronics and Communication Engineering, Goel Institute of Management and Technology, Lucknow, Uttar Pradesh, India.

²Associate Professor, Department of Electronics and Communication Engineering, Goel Institute of Management and Technology, Lucknow, Uttar Pradesh, India.

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necessitate the use of additional energy sources. Renewable electricity is celebrated for being affordable, accessible, and free from greenhouse gas emissions. One practical solution is photovoltaic cells, which turn sunshine into electricity. Over the past two decades, numerous material opportunities have enabled scientific advancements in photovoltaic technology, lowering costs and enhancing solar cell efficiency. In 1954, Bell Laboratories developed the first efficient photovoltaic system, achieving 6% efficiency. Silicon solar panels with a 1 eV band gap tend to be more efficient. Lightweight film solar cells offer advantages due to their low weight and flexibility. Third-generation solar cells often use materials like organic dyes, conductive polymers, and silicon wire, with larger band gaps. The development of

photovoltaic cells is expected to be crucial for the future of renewable energy sources. They offer an endless supply without emitting carbon dioxide. Sustainable energy can be generated using natural resources like sunlight, tides, wind, and rain. Solar energy is safe and beneficial for health, homes, and businesses. In the future, solar cells might become the primary renewable energy source. Currently, solar power is the most reliable and stable form of free energy. Various elements within the perovskite family could significantly impact this field. Copper Iodide (CuI) is advantageous due to its chemical stability, ease of synthesis, and high transparency in the visible spectrum. However, processing CuI in Deep Eutectic Solvents (DES) can cause the perovskite layer to degrade. Researchers have attempted to create CuI-based PSCs with p-in configurations [1–8]. In 2015, Ye *et al.* rapidly deposition-crystallized a CH₃NH₃PbI₃ film with X=I, Br, and Cl after electrodepositing a CuI layer [3]. The average PCE was 15%, with a peak PCE of 16.6%. CuI-based PSCs achieved a 6% success rate, likely due to the high hole mobility of the Cu(H)CN HTL. This was facilitated by the low interface resistance and smoothness of the perovskite films [9]. Additionally, unconventional methods have been used to create the perovskite layer. The effectiveness of the HTL in CH₃NH₃PbI₃, X=I solar cells made from perovskite and inorganic copper iodide (CuI), has been investigated. A solar cell, through the photovoltaic effect. Here is a simplified explanation of how a solar cell works:

1. *Sunlight absorption:* Typically, silicon and other semiconductor-related materials are used to create solar cells. The semiconductor substance in the solar cell absorbs part of the photons in sunlight that strike its surface.
2. *Creation of electron-hole pairs:* After photons are absorbed, they impart their energy to semiconductor electrons, causing them to reach higher energy states. As a result, pairs of electrons with free-moving electrons are created, leaving the material with positively charged “holes” in it.
3. *Charge carrier separation:* The charge carriers are separated by the internal electric field in the semiconductor material, which causes the positively charged holes and free electrons to go in opposing directions.
4. *Charge carrier collection:* The separation of electrons and holes is made easier by metal contacts that are placed on the top and bottom surfaces of the solar cell. Through these connections, current, or electrons, can leave the cell and be used for external electrical applications.
5. *Conversion of light energy to electrical energy:* The flow of electrons through an external circuit that is connected to a solar cell produces an electric current. The amount of current can be used to power electric equipment and may also be preserved in batteries for future use.
6. *Operation in closed circuit:* The electrons continue to flow via the external circuit if sunlight is present, and the circuit is closed. Nevertheless, the flow of electrons stops when the circuit is opened, or sunlight is blocked.

Essentially, a solar cell is a sustainable and renewable source of electricity that converts the energy from sunshine into an electric current [10]. Solar panels, which can be used for commercial, industrial, or residential purposes, can generate more electricity by connecting several solar cells.

PEROVSKITE MATERIAL

Especially in the field of solar energy, perovskite materials are an intriguing class of chemicals that stand out for their many uses. Perovskites are well-known for their unique crystal structure and adaptable nature, and they have several notable features and qualities.

Crystallographically speaking, perovskites use the general formula ABX₃, in which the anion is represented by 'X' and the cations by 'A' and 'B', the former of which is usually larger than the latter. Depending on the surroundings, its crystal structure can take the form of cubic, tetragonal, or orthorhombic formations [11–14].

Their remarkable optical absorption properties, which include significant absorption and a tenable band gap, two essential characteristics supporting their effectiveness in solar applications, are noteworthy. Perovskites are excellent at charge transport; they have long diffusion lengths, ambipolar

charge mobility, and high carrier mobility, all of which are essential for effective energy conversion. Moreover, they have a strong resistance to point faults, which improves stability and performance, a feature that is very useful in a variety of applications.

Some forms of perovskite, especially those that contain cobalt, show magnetic characteristics that can be attributed to the intrinsic spin of cobalt. Furthermore, perovskite properties, both optical and electrical, can be precisely adjusted to meet needs by doping, a procedure that involves the introduction of impurities.

These materials can be roughly divided into two groups: pure inorganic perovskites, which are represented by compounds such as PbTiO_2 and CaSiO_2 , and hybrid organic-inorganic perovskites, which are represented by compositions like $\text{CH}_3\text{NH}_3\text{MX}_3$ (where $\text{M}=\text{Pb}$ or Sn ; $(\text{X}=\text{I})$).

ADVANTAGES OF PEROVSKITE MATERIALS

1. *High efficiency:* Perovskite solar cells promise affordable solar energy generation due to their competitive efficiency.
2. *Tenable properties:* Their adaptable bandgap enables customized optical and electrical properties, improving adaptability in a range of applications.
3. *Plenty and low-cost production:* Perovskite materials, which are made up of plenty of inexpensive elements, have the potential to be produced in large quantities using low-cost production techniques.
4. *Versatility:* Because of its various forms and characteristics, perovskite materials are used in applications other than solar cells, such as LEDs, sensors, and light detectors.

DISADVANTAGES OF PEROVSKITE MATERIALS

1. *Stability concerns:* Limited in terms of long-term dependability and economic viability due to susceptibility to deterioration when exposed to moisture, oxygen, and light.
2. *Toxicity issues:* Lead is present in some formulations, which poses health and environmental risks during production, use, and disposal.
3. *Scaling challenges:* Commercial adoption is hampered by difficulties in sustaining consistent quality and efficiency during large-scale production.
4. *Material reproducibility:* Differences in synthesis methods and processing circumstances make it difficult to achieve consistent performance across batches.

FUTURE SCOPE OF PEROVSKITE MATERIALS

1. *Perovskite solar cell commercialization:* Research aims to improve scalability and stability for broad usage in solar energy generation.
2. *Examining lead-free substitutes:* Research endeavors are focused on creating environmentally sustainable compositions to tackle health issues and increase market acceptability.
3. *Expanding into new technologies:* Perovskite materials are being researched for use in LEDs, sensors, and optoelectronic devices, among other uses besides photovoltaics.
4. The focus of efforts is on ensuring a smooth integration of perovskite technologies with well-established semiconductor platforms to maximize performance and take advantage of synergies.

APPLICATIONS OF PEROVSKITE MATERIALS

1. *Solar energy:* A viable substitute for conventional silicon-based solar cells, perovskite solar cells use sunlight to produce power.
2. *LEDs and lighting:* Perovskite materials are a good fit for LED technologies since they can emit light in an efficient and sustainable manner [15].
3. *Sensors and photo detectors:* Due to their great sensitivity and responsiveness, perovskite-based sensors and photo detectors find use in biomedical equipment, security systems, and environmental monitoring.

4. *Optoelectronic devices*: Because of its superior optical and electrical qualities, perovskite materials are used in a variety of optoelectronic devices, such as lasers, screens, and detectors.

FABRICATION OF PEROVSKITE SOLAR CELL

The “planar heterogeneous junction” structure and perovskite photovoltaic cells (PSCs) have similar designs. The electron transport layer is made of silicon dioxide (SiO₂), while the glass substrate layer consists of transport conducting oxides (TCO). In perovskite materials, CuI functions as the hole transport layer (HTL) for the metal back contact, and CH₃NH₃PbI₃, X=I, serves as the active layer.

Photovoltaic cells rely on the photovoltaic effect to generate electricity from sunlight without emitting gases like carbon dioxide or other pollutants such as sulfur or nitrogen. Solar cells can also indirectly convert solar energy into electricity by first transforming it into heat or chemical energy, posing no risks to the environment or human health [16–19]. These cells are low-maintenance, durable, and can be easily installed in various locations, including homes, workplaces, caravans, tourist attractions, calculators, watches, light meters, and cameras. They offer a silent, non-infectious, economical, eco-friendly power source that is also non-polluting [20–23].

Global warming is a severe threat to humanity and wildlife on Earth. During the 19th century, sea levels rose by 10–25 cm, and surface temperatures increased by 0.3–0.6°C due to global warming. Rising sea levels have led to more severe natural disasters and significant disruptions to human life and ecosystems.

Numerous tiny cells are used in solar panels to produce a certain level of power. Current solar cell technologies aim to create electrons and holes in each cell. CuI acts as the HTL for the metal back contact, and CH₃NH₃PbI₃, a perovskite material, forms the active layer. Using CuI as the HTL in perovskite solar cells improves their efficiency. Research indicates that spiro-MeOTAD has a higher fill factor (FF) but lower electrical conductivity than CuI as shown in Figure 1.

The impressive power conversion efficiency (PCE) of 16.6% achieved by CuI-based PSCs, exceeding the median PCE of 15.6%, is likely due to the high hole mobility of the CuI HTL. The low surface roughness and interface resistance of the resulting perovskite films also contributed to this efficiency [24, 25]. Furthermore, specially designed methods have effectively reduced the degradation of the perovskite layer caused by the synthesis of CuI in the n-i-p PSC solution, where the active layer is CH₃NH₃PbI₃, X=I.

PARAMETERS OF A SOLAR CELL

1. *Efficiency*: This measures how much sunlight is converted into usable electricity. It is critical because higher efficiency means more power from the same amount of sunlight.
2. *Open-circuit voltage (Voc)*: The maximum voltage a solar cell can produce when not connected to a load. This voltage exists when no current is flowing.

Black metal contact
Hole transport layer (0.100, 0.200, 0.300 μm)
Absorber layer (CH ₃ NH ₃ PbX ₃ , X: I) (0.35 μm)
Electron transport layer (0.030 μm)
Transparent conducting oxide (0.500 μm)
Glass substrate

Figure 1. Fabrication of solar cell using perovskite material.

3. *Short-circuit current (ISC)*: The highest current a solar cell can produce when its terminals are shorted, meaning the voltage is zero.
4. *Fill factor (FF)*: This value shows how close the solar cell comes to achieving its maximum power output. It is calculated by dividing the cell's actual power by the product of its open-circuit voltage, short-circuit current, and the voltage and current at the maximum power point.
5. *Maximum power point (Pmax)*: The point on a solar cell's current-voltage (I-V) curve where the product of current and voltage is at its peak, indicating the cell's maximum power output under given conditions.
6. *Temperature coefficient*: This shows how temperature changes impact the solar cell's performance. Typically, efficiency decreases as temperature rises.
7. *Shunt resistance (Rsh)*: This is the resistance parallel to the p-n junction of the solar cell, representing the path of leakage current.
8. *Series resistance (Rs)*: This is the resistance in series with the p-n junction of the solar cell, accounting for resistive losses within the cell.

RESULTS AND DISCUSSION

The perovskite cell $\text{CH}_3\text{NH}_3\text{PbX}_3$ (X: I) performance metrics, which include J_{sc} , FF, V_{oc} , C-F, C-V, and PCE, are listed in Table 1. The cell's efficacy has been demonstrated. For the simulation, two illumination settings are used: low and high. When employing CuI to transfer holes and layer, the outcomes diverge from those observed by other searchers. Every perovskite solar cell material that has been researched has a working point voltage of 0 V in the dark and 0.5 V in the light. Table 1 contains a list of the various determined features for the perovskite solar cell under investigation.

Comparing the $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell to those of other researchers, at the thickness of 0.100 μm , the simulated findings show parameters for performance such $V_{oc}=1.837$, $J_{sc}=28.82$, $FF=89.59$, and $PCE=29.54$ watts.

At the thickness of 0.200 μm the simulated findings show parameters for performance such as $V_{oc}=1.837$ V, $J_{sc}=28.82$, $FF=85.64$, and $PCE=29.22$ watts. Also, at the thickness of 0.300 μm the simulated findings show parameters for performance such $V_{oc}=1.3408$ V, $J_{sc}=28.82$, $FF=74.96$, and $PCE=28.97$ watts. Further, Figures 2 and 3 graphs show all the output for the provided parameters by varying the thickness of the HTL (Hole Transport Layer) as CuI (Copper Iodide). For the $\text{CH}_3\text{NH}_3\text{PbX}_3$ (X: I) perovskite solar cell, the current density (JV) characteristics were calculated as seen in Figure 2. For the $\text{CH}_3\text{NH}_3\text{PbX}_3$ (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 Figure 3.

For the $\text{CH}_3\text{NH}_3\text{PbI}_3$ 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 $\text{CH}_3\text{NH}_3\text{PbI}_3$ is more responsive to capacitance production at higher frequency ranges.

For a $\text{CH}_3\text{NH}_3\text{PbI}_3$ based solar cell, the variation in capacitance (nFcm^{-2}) is measured according to the applied voltage, and it increases exponentially with respect to voltage. For $\text{CH}_3\text{NH}_3\text{PbI}_3$, the capacitance (nFcm^{-2}) rises and at thickness 0.100 of HTL saturated. Figure 5 plots the calculated capacitance (C) vs. voltage (V) for the perovskite solar cell under investigation.

Table 1. The variously computed characteristics of the perovskite solar cell under study ($\text{CH}_3\text{NH}_3\text{PbX}_3$, X: I).

Hole transport layer as copper iodide (CuI)	Parameter			
	V_{oc} (V)	J_{sc} (mAcm^{-2})	FF	PCE (%)
At thickness 0.100 μm	1.837	28.82	86.59	29.54
At thickness 0.200 μm	1.837	28.82	85.64	29.22
At thickness 0.300 μm	1.3408	28.82	74.96	28.97

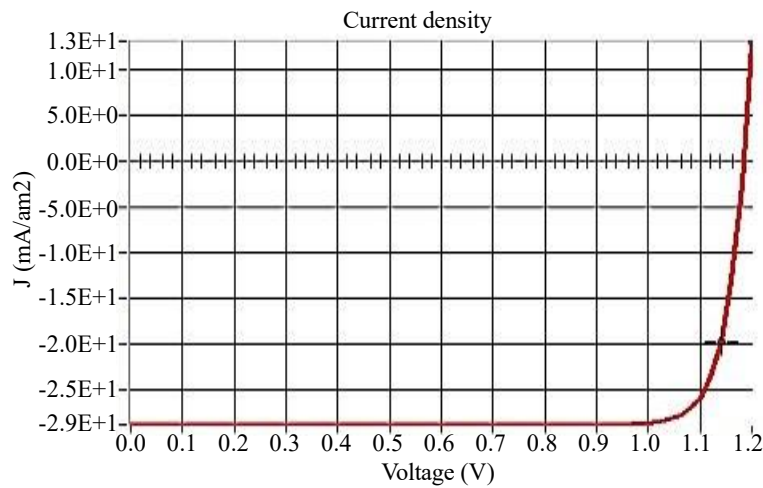


Figure 2. The J-V characteristics for the $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at thickness 0.100 of HTL.

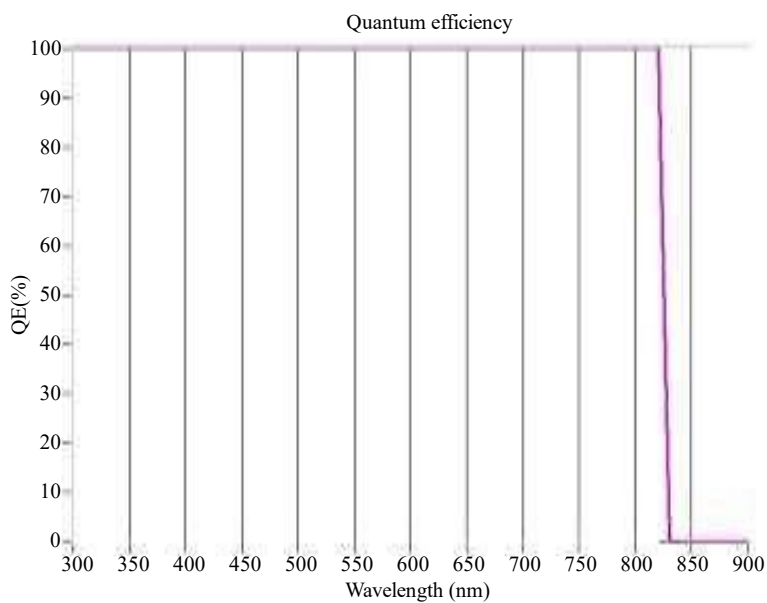


Figure 3. Quantum efficiency of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar.

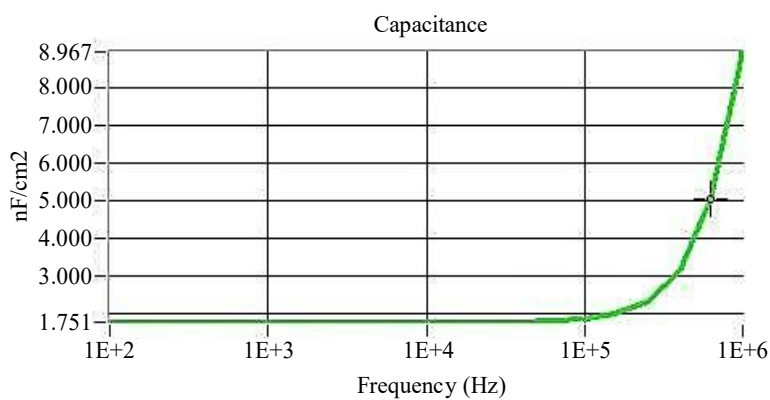


Figure 4. C-f characteristics for $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at thickness 0.100 of HTL.

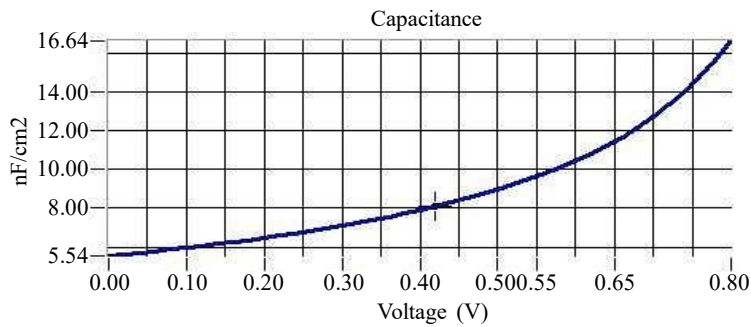


Figure 5. The C-V characteristics of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at thickness 0.100 of HTL.

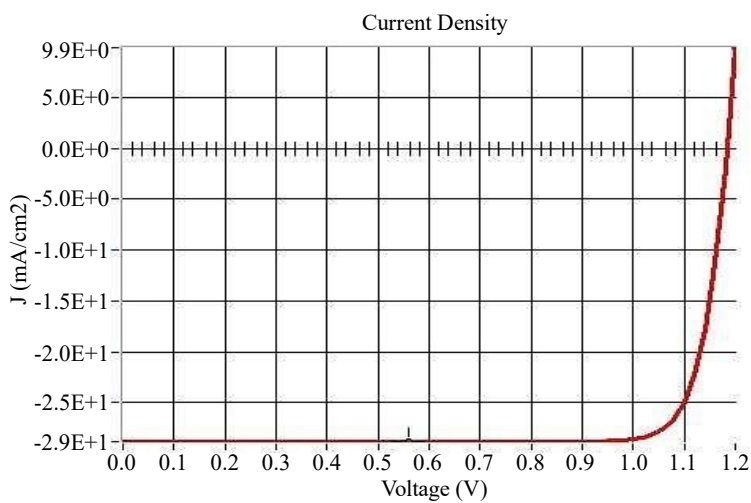


Figure 6. The J-V characteristics for the $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at HTL thickness 0.200 μm .

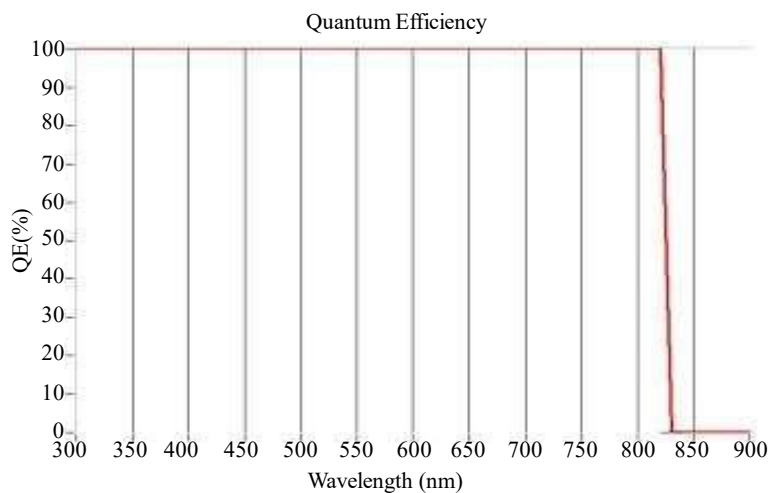


Figure 7. Quantum efficiency of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at HTL thickness 0.200 μm .

For the $\text{CH}_3\text{NH}_3\text{PbX}_3$ (X: I) perovskite solar cell, the current density (JV) characteristics at thickness 0.200 of HTL were calculated as seen in Figure 6. For the $\text{CH}_3\text{NH}_3\text{PbX}_3$ (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 Figure 7, at thickness 0.200 of HTL.

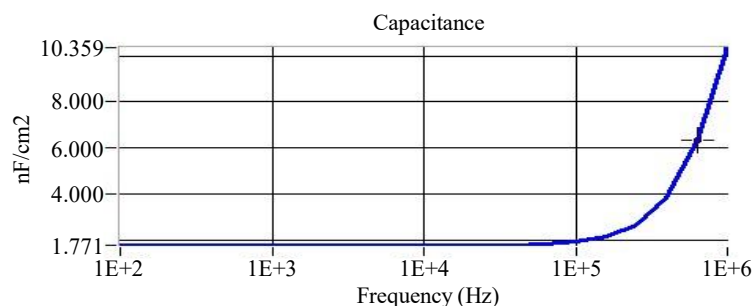


Figure 8. C-f characteristics for $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at HTL thickness $0.200 \mu\text{m}$.

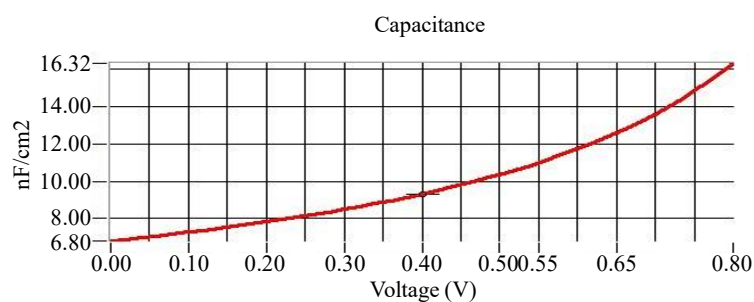


Figure 9. The C-V characteristics of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at HTL thickness $0.200 \mu\text{m}$.

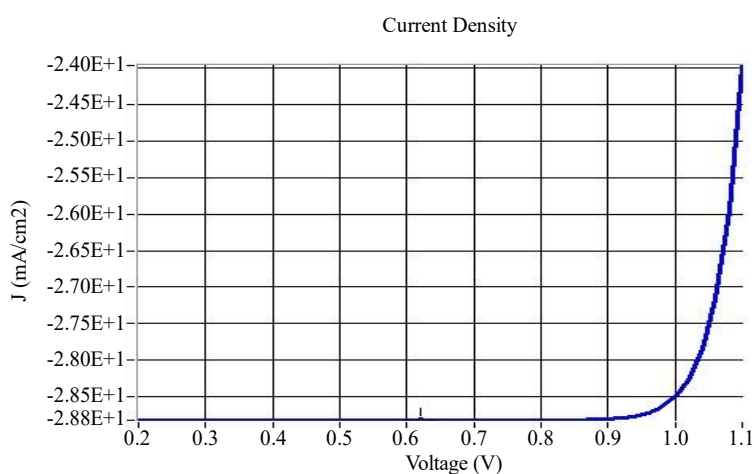


Figure 10. The J-V characteristics for the $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at HTL thickness $0.300 \mu\text{m}$.

For the $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell under study, the capacitance-frequency (C-f) properties have been determined and are displayed in Figure 8 at thickness 0.200 of HTL. By adjusting the alternating current signal frequency during the C-f measurements, capacitance is computed. This demonstrates that $\text{CH}_3\text{NH}_3\text{PbI}_3$ is more responsive to capacitance production at higher frequency ranges.

For a $\text{CH}_3\text{NH}_3\text{PbI}_3$ based solar cell, the variation in capacitance (nFcm^{-2}) is measured regarding the applied voltage, and it increases exponentially with respect to voltage at thickness 0.200 of HTL. For $\text{CH}_3\text{NH}_3\text{PbI}_3$, the capacitance (nFcm^{-2}) rises and becomes saturated. Figure 9 plots the calculated capacitance (C) vs. voltage (V) for the perovskite solar cell under investigation. For the $\text{CH}_3\text{NH}_3\text{PbX}_3$ (X: I) perovskite solar cell, the current density (JV) characteristics were calculated as seen in Figure 10 at thickness 0.300 of HTL.

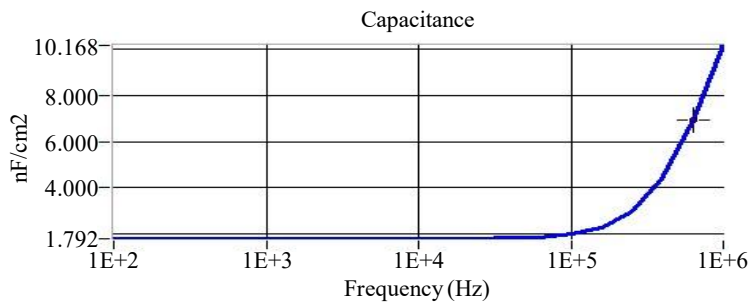


Figure 11. C-f characteristics for $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at HTL thickness $0.300 \mu\text{m}$.

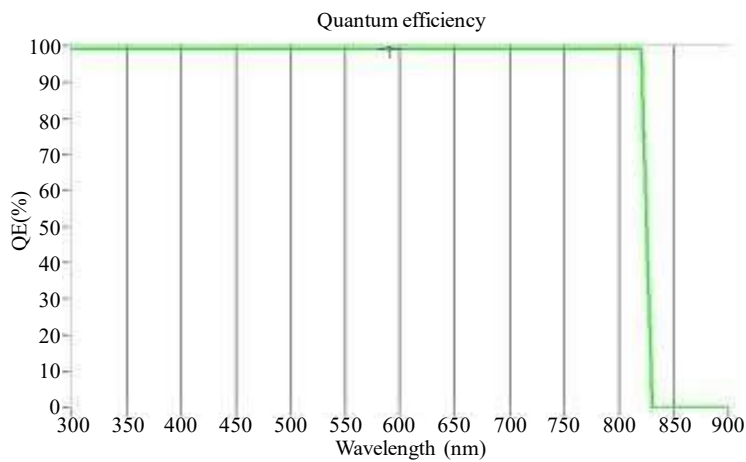


Figure 12. Quantum efficiency of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar.

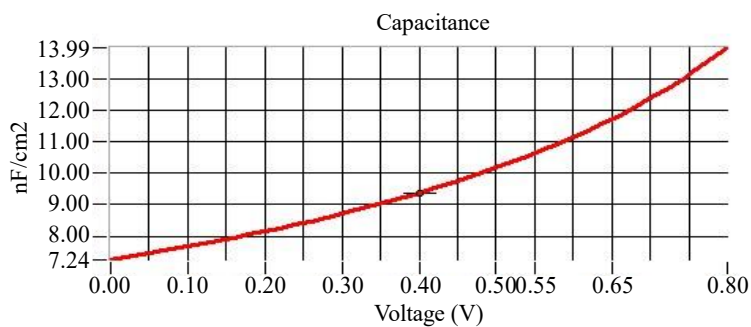


Figure 13. The C-V characteristics of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell at HTL thickness $0.300 \mu\text{m}$.

For the $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell under study, the capacitance-frequency (C-f) properties have been determined and are displayed in Figure 11 at thickness $0.300 \mu\text{m}$ of HTL. By adjusting the alternating current signal frequency during the C-f measurements, capacitance is computed. This demonstrates that $\text{CH}_3\text{NH}_3\text{PbI}_3$ is more responsive to capacitance production at higher frequency ranges.

For the $\text{CH}_3\text{NH}_3\text{PbX}_3$ (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 Figure 12 at thickness $0.300 \mu\text{m}$ of HTL.

For a $\text{CH}_3\text{NH}_3\text{PbI}_3$ based solar cell, the variation in capacitance (nFcm^{-2}) is measured regarding the applied voltage, and it increases exponentially with respect to voltage at thickness $0.300 \mu\text{m}$ of HTL. For $\text{CH}_3\text{NH}_3\text{PbI}_3$, the capacitance (nFcm^{-2}) rises and becomes saturated. Figure 13 plots the calculated capacitance (C) vs. voltage (V) for the perovskite solar cell under investigation.

CONCLUSION

In the present investigation, the hole transport layer (HTL) and the solar cell simulator software (SCAPS) Tool are used to evaluate the performance of solar cells employing perovskite material, such as CH₃NH₃PbI₃. The fill factor (FF), short-circuit current density (J_{sc}), power conversion rate (PCE), and open-circuit voltage (V_{oc}) of the MAPbI₃ material employed for the active layer have all been determined using quantitative simulation and modelling. The capacitance-frequency (C-F) and capacitance-voltage (C-V) of the previously examined solar cell made of perovskite have been calculated. The solar cell simulation software (SCAPS) Tool demonstrates that the hole transport layer (HTL) is essential for the efficiency of solar cells employing perovskite materials like CH₃NH₃PbI₃. The electrical characteristics of MAPbI₃ material in the active layer of the semiconductor have been ascertained using quantitative computations and models, with particular attention to variables such as fill factor (FF), power conversion efficiency (PCE), short-circuit current density (J_{sc}), and open-circuit voltage (V_{oc}). The capacitance-frequency (C-F) and capacitance-voltage (C-V) of previously researched perovskite solar cells have been calculated. According to the simulation results, MAPbI₃ at various HTL thicknesses yields FF=86.59, PCE=29.54 watts, V_{oc}=1.1837 V, and J_{sc}=28.82 mA/cm² at the 0.100 thickness; FF=85.64, PCE=29.22 watts, V_{oc}=1.1837 V, and J_{sc}=28.82 mA/cm² at the 0.200 thickness; additionally, at 0.300 thickness, FF=74.96, PCE=28.97 watts, V_{oc}=1.3408 V, and J_{sc}=28.82 mA/cm² are provided.

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