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Design of Lead-Free Perovskite ($CH_3NH_3SnX_3$, X=I) Solar Cell Using SCAPS-1D

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Abstract

Research on renewable energy conversion technology has accelerated due to the world's growing energy needs. Researchers from all over the world are interested in lead-based perovskite materials. These cells are being developed as a substitute for conventional solar cells because they have the potential to increase solar energy conversion efficiency. Lead's advantageous electrical and optical characteristics make it a viable option for photovoltaic and optoelectronic applications. Lead's limited material stability and poisonous nature, however, limit its potential for use in new products. In order to avoid lead, researchers are concentrating on creating environmentally benign perovskite solar cells. Using lead-free perovskite material such as methyl ammonium tin trihalide ($MASnX_3$, MA = CH_3NH_3, X = I) and SCAPS (Solar Cell Capacitance Simulator) tools, extensive modeling and numerical simulation of perovskite solar cells were conducted. Measurements such as open-circuit voltage (V_{oc}), fill factor (FF), power conversion efficiency (PCE), along with short-circuit current density (J_{sc}) of the MASnI3 material used as active layer, respectively were performed. In the envisioned structure of the perovskite solar cell, the copper thiocyanate (CuSCN) molecule plays a crucial role as a hole transmitting layer. The featured structure parameters for $CH_3NH_3SnI_3$ are a FF of 14.76, a PCE of 30.69%, aV_{oc} of 6.7060, along with a J_{sc} of 30.9950 mA/cm^2, according to the findings of the simulation.

Keywords: Perovskite solar cell, CuSCN, fill factor (FF), open circuit voltage (V_{oc}), short-circuit current density (J_{sc}), power conversion efficiency (PCE), capacitance-voltage (C-V) characteristics, capacitance-frequency (C-F) characteristics, $CH_3NH_3SnI_3$

INTRODUCTION

Lead-free perovskite solar cells, particularly those based on tin (Sn) instead of lead (Pb), have emerged as a promising alternative to traditional lead-based perovskites due to their potential for reducing toxicity concerns while maintaining high photovoltaic performance. Methyl-ammonium tin iodide ($CH_3NH_3SnI_3$) is one such material that has attracted significant attention due to its favorable optical and electronic properties. These lead-free perovskites offer a safer and more environmentally friendly option for next-generation solar cells. SCAPS-1D (Solar Cell Capacitance Simulator in 1 Dimension) is a powerful simulation tool used to model and optimize the performance of such devices by simulating charge transport, recombination, and the overall electrical behavior of the solar cell [1–4]. By adjusting key parameters such as material properties, layer thicknesses, doping concentrations, and defect densities, SCAPS-1D allows researchers to design and optimize lead-free perovskite solar cells for maximum efficiency. This approach can help accelerate the development of sustainable, high-performance solar technologies. The growing concern over the environmental impact of lead-based materials has driven significant research into lead-free alternatives for perovskite solar cells.

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Among these alternatives, methyl-ammonium tin iodide ($CH_3NH_3SnI_3$) has gained considerable attention due to its promising optoelectronic properties, including a suitable band-gap (~1.3–1.4 eV), high absorption coefficient [5], and potential for low-cost production. While tin-based perovskites are less toxic than their lead counterparts, they still face challenges such as lower stability and efficiency, which require careful design and optimization. SCAPS-1D plays a crucial role in addressing these challenges by offering a comprehensive platform for simulating the behavior of lead-free perovskite solar cells. The software allows for the investigation of various device parameters, such as material selection, layer thicknesses, doping levels, and defect densities, which significantly impact the solar cell's efficiency and stability [6–10]. By adjusting these parameters and simulating device performance under different conditions, SCAPS-1D enables researchers to fine-tune the design of lead-free perovskite solar cells, aiming to achieve high power conversion efficiencies while minimizing material-related issues. This modeling approach not only accelerates the development of lead-free technologies but also supports the transition towards more sustainable and environmentally friendly solar energy solutions. Traditionally, fossil fuels have been vital since the first industrial revolution and continue to be a primary factor behind modern society. Previous industrial revolutions brought about an unequaled period of wealth for human society, but they also increased the dispute between humans and nature, led to immense resource consumption and increased energy costs, and resulted in enormous ecological and costs to the environment [11]. Conventional fossil fuels cannot meet the growing demand for energy, which has been accelerating along with the world economy and the social forces driving it. The global crises of ecology, resource extraction and distribution, the environment, and climate change have left humanity facing unprecedented challenges as we move into the twenty-first century. All of these issues have sparked the start of the fourth industrial revolution, sometimes known as the green industrial revolution. These days, with solar energy being the primary energy source, it will unavoidably provide new means of support for the advancement of humanity and society because of its many benefits, including being pollution-free, renewable, and extremely powerful. One of the primary applications of solar energy, optoelectronic conversion, has been extensively studied in the past few decades. Among the most important kinds of optoelectronic converters are solar cells. The development of low-cost, high-efficiency solar cells has gained prominence in recent years. Perovskite solar cells (PSCs) are a promising class of solar cells that have garnered a lot of attention in the last ten years due to their improved bipolar charge mobility, high absorption coefficient, low trap state density, diminished exciton binding energy, expanded carrier diffusion length, as well as adjustable band-gap [12–14].

The power conversion efficiency (PCE) of PSCs based on lead perovskites has grown dramatically, from 3.8% to a recently approved figure of 30.69%. However, there are some unavoidable disadvantages associated with these Pb-based high-efficiency PSCs ($MAPbI_3$, $FAPbI_3$, Cs0.05FA0.85MA0.10Pb $(I0.97Br0.03)_3$), such as the fact that lead is toxic to living beings and the environment and that it makes it hard for the body to eliminate. Research indicates that lead ions permanently contaminate the water and soil supplies, which is extremely harmful to the survival of plants, animals, and people [15]. Lead poisoning causes functional anomalies in the human body's mental, gastrointestinal, and blood systems over time. This is because lead enters the human body during blood circulation, forms a connection to a digestive enzyme, and then builds up in connective tissue and bones such as the brain, kidney, liver, and spleen. Most people frequently display signs of lead poisoning when their daily lead exposure reaches approximately 0.5 mg. In order to protect people and maintain a clean environment, some non- or low-toxic metal ions must be developed to replace lead as perovskite absorbers of PSCs.

A variety of additional elements within such a structure could greatly improve the perovskite family. Apart from the aforementioned benefits, CuSCN exhibits remarkable transparency within the noticeable spectrum, affluence of amalgamation, and robust chemical stability. Nevertheless, the perovskite layer may deteriorate if CuSCN is processed in solutions using the conventional diethyl sulfide (DES) solvents. Consequently, scientists tried to produce CuSCN-based PSCs using a p-i-n arrangement. CuSCN was electrodeposited, and a film of $CH_3NH_3SnX_3$, X = I, was rapidly deposition-crystallized on top of that layer. A median PCE of 15.6% and an exceptional PCE of 16.6% were achieved by the

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CuSCN-based PSCs; this may also be connected to the remarkably high hole mobility for CuSCN hole transport layer (HTL). The small interface resistance to contact and low apparent coarseness of the resulting perovskite films allowed for this. Furthermore, it has been shown that the erosion of the perovskite layer resulting from the production of CuSCN in the solution for n-i-p PSCs may be effectively reduced by employing particular unique techniques. This study examines the performance of $CH_3NH_3SnX_3$, X = I solar cells utilizing inorganic copper thiocyanate (CuSCN) as the HTL.

FABRICATION OF SOLAR CELL USING PEROVSKITE MATERIAL

The architecture of the "planer heterogeneous junction" and lead-free PSC are identical. The glass substratum layer comprised of transparent conductive oxides (TCOs) and the transport electron layer consisting of titanium dioxide (TiO_2). In perovskite materials, the active layer is represented by X = I and $CH_3NH_3SnX_3$, with CuSCN acting as the HTL for metal reverse contact.

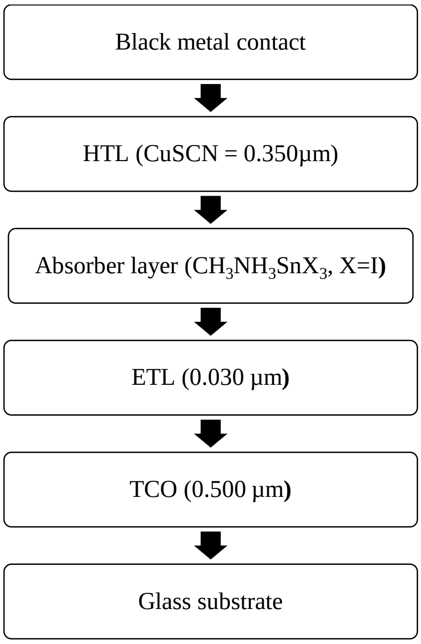

Figure 1. Representation of perovskite solar cell.

Table 1. SCAPS simulation parameter of $CH_3NH_3SnI_3$.

Parameters	**TCO**	**ETL**	**Absorber ($CH_3NH_3PbI_3$)**	**CuSCN (HTL)**
Thickness (µm)	0.50	0.030	0.10	0.350
Band gap (eV)	3.5	3.2	1.3	3.6
Electron affinity (eV)	4	4.26	4.7	1.7
Relative permittivity	9	38	6.5	7.1
Conduction band density (cm^{-3})	2.00×10^{18}	2.00×10^{18}	1.00×10^{18}	2.2×10^{19}
Valance band density (cm^{-3})	1.80×10^{19}	1.80×10^{19}	1.00×10^{18}	1.80×10^{18}
Electron mobility ($cm^2V^{-1}s^{-1}$)	20	2	1.6	10
Hole mobility ($cm^2V^{-1}s^{-1}$)	50	2	1.6	25
Donor concentration (cm^{-3})	2.00×10^{19}	1.00×10^{16}	0	0
Acceptor concentration (cm^{-3})	0	0	3.2×10^{21}	1.00×10^{18}
Defect density (cm^{-3})	1.00×10^{15}	1.00×10^{15}		
Capture cross section for electrons (cm^2)	2.0×10^{-15}	1.00×10^{-15}	2.00×10^{-14}	1.00×10^{-15}
Capture cross section for holes (cm^2)	2.0×10^{-15}	1.00×10^{-15}	2.00×10^{-14}	1.00×10^{-15}

ETL, electron transport layer; TCO, transparent conductive oxide.

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CuSCN is the HTL enabling the metallic back contact, and $CH_3NH_3SnI_3$ from the thermoelectric family makes up the active layer. In perovskite solar cells, CuSCN material serves as the HTL, optimizing the cell's efficiency. Impedance spectroscopy results [15–17] show that the spiro-MeOTAD differs from CuSCN in that it has a smaller electrical conductivity level and a substantially larger fill factor (FF).

RESULTS AND DISCUSSION

To improve solar cell efficiency and free toxic in nature, a type of lead-free perovskite structure of cells called $CH_3NH_3SnI_3$, has been modernized [18–21]. J_{sc}, FF, V_{oc}, and PCE have also been measured as performance metrics as shown in Figures 2 to 5. Both dim and strong lighting are used to perform the simulation [22–26].

Whenever there is no light, the voltage at the working point is 0. For each solar cell comprised of perovskite elements in the low illumination state, the simulation is set to 0.5V. The numerous perovskite solar cells are listed in Table 2 along with the measurements made for each of their unique features.

Figure 2 displays the J-V parameters for the perovskite solar cell under examination. Figure 3 demonstrates the features of the quantum efficiency (QE) for the $CH_3NH_3SnI_3$ lead-free perovskite solar cells. The capacitance-frequency (C-F) characteristics for the lead-free perovskite solar cell $CH_3NH_3PbI_3$, are plotted and shown in Figure 4. The C-V characteristics for the perovskite solar cells $CH_3NH_3SnI_3$ are plotted and shown in Figure 5.

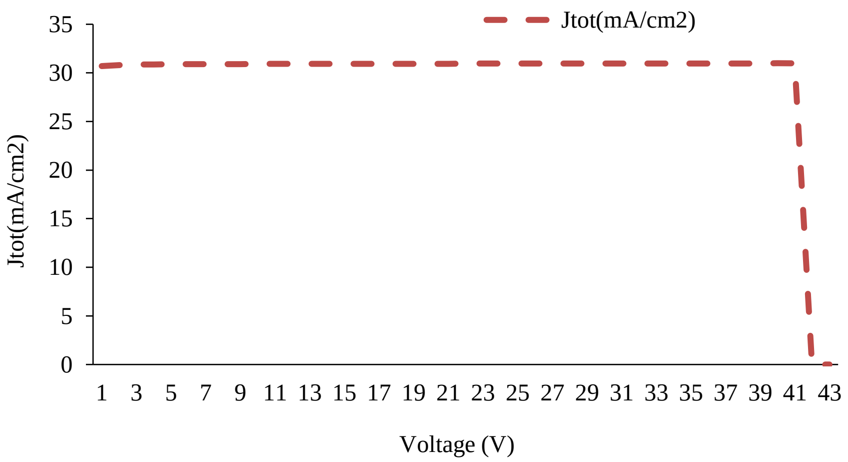

Figure 2. J-V characteristics for the lead-free perovskite solar cell.

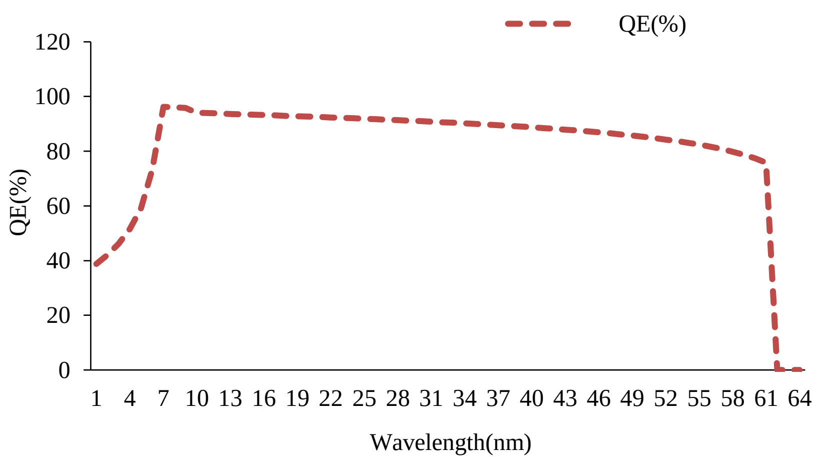

Figure 3. Quantum efficiency of $CH_3NH_3SnI_3$, lead-free perovskite solar cell.

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Table 2. Various premeditated parameters for intentional perovskite solar cell.

Material		Parameter			
		V_{oc} *(V)*	J_{sc} *(mA/cm^2)*	*Fill Factor (FF)*	*Power Conversion Efficiency (PCE) (%)*
$CH_3NH_3SnI_3$	Previous work	0.989	33.86	66.33	22.21
$CH_3NH_3SnI_3$	Present work	6.7060	30.9956	14.76	30.69

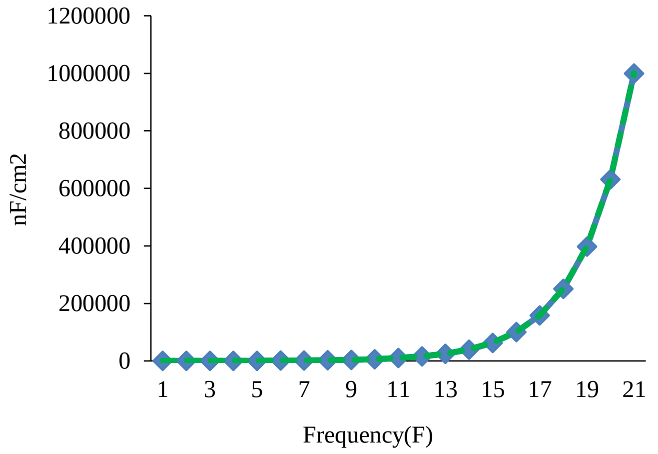

Figure 4. Capacitance-frequency (C-F) characteristics of $CH_3NH_3SnI_3$ lead-free perovskite solar cell.

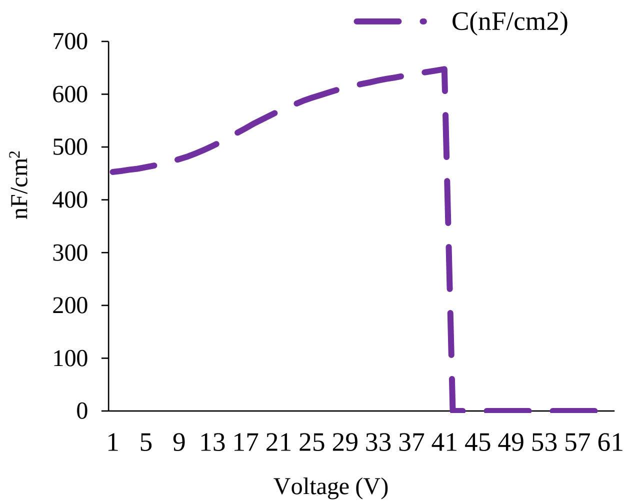

Figure 5. Capacitance-voltage (C-V) characteristics of $CH_3NH_3SnI_3$, lead-free perovskite solar cell.

CONCLUSION

The world's expanding energy needs have driven research into renewable energy conversion technologies. Lead-based perovskite materials are of interest to researchers worldwide. Lead is a good choice for both photovoltaic and electronic applications because of its beneficial electrical and optical properties. Nonetheless, the low material stability and toxic nature of lead restrict its application in novel products. According to simulation findings the $CH_3NH_3SnI_3$ material like a fill factor (FF) of 14.76, PCE of 30.69 %, with V_{oc} of 6.7060 V, and J_{sc} of 30.9956 mA/cm^2.

The copper thiocyanate (CuSCN) molecule serves as a critical HTL in the lead-free perovskite solar cell's proposed structure and play important role in term of power conversion efficiency. The $CH_3NH_3SnI_3$ material is shows better results with respect to other material which are used in the cells.

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