Optimization of Conversion Efficiency of Perovskite Solar Cell using Cu_2O and CuI as Hole Transport Layer

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Abstract:

Nowadays solar cells are a prominent technology and play a vital role in the future of renewable energy sources for human society. The primary challenge is to make these solar cells to the reach of human society. In this price-competitive market, solar technologies must be cheap and efficient. Perovskite solar cells can be a better solution for this purpose. These perovskite solar cells are cheaper than the traditional inorganic solar cells but the power conversion efficiency (PCE) improvement is still an open area to work on. The PCE depends on various parameters like hole transport layer (HTL) material, the absorber layer, absorption coefficient, and the thickness of the absorber. The price of solar cells is determined by the HTL materials. The use of low-cost HTL materials is preferred. Using Copper Iodide (CuI) and Cuprous Oxide (Cu_2O) as HTL materials, this research looked at and improved the PCE of perovskite solar cells ($CH_3NH_3PbX_3$, X: I, Br, Cl). Cu_2O and CuI are utilized as the HTL in perovskite solar cells and have a major impact on PCE as well as other metrics like open-circuit voltage, fill factor, and short circuit current density. With $CH_3NH_3PbX_3$, X: I, Br, Cl materials, the C-F and C-V physical properties are also investigated. The thickness of the active Layer ($CH_3NH_3PbI_3$) is also thought to play a role in the stability and efficiency of perovskite solar cells. The SCAPS programme is used to perform simulations and thorough modeling on perovskite solar cells employing perovskite material such as Methyl Ammonium Lead Iodide ($MAPbI_3$, $MA=CH_3NH_3$) at various thicknesses. The $CH_3NH_3PbI_3$ perovskite solar cell with HTL of Cu_2O has a higher open circuit voltage, short circuit current density (Jsc), fill factor, and PCE than other perovskite materials. CuI, on the other hand, is a significant HTL material. Our testing results show that the PCE of solar cells is 20.95, which is significantly higher than prior research findings, which ranged from 6% to 17%.

Key Word*: PCE, Perovskite Solar Cell, HTL.*

I. Introduction

Solar energy reaches the Earth in large amounts. The sun produces enough energy each minute to meet the world's energy needs for a whole year, and one day produces more energy than the entire population of the planet. Solar cells are a promising technology with significant implications for the future of renewable energy and human society. Sustainable energy is a limitless source of energy that is conveniently accessible and does not emit CO_2. Sustainable energy is generated from natural sources such as the sun, tides, wind, and rain and maybe produced repeatedly when needed.There are three generations of solar cells: first, second, and third. In comparison to the first and second generations, the third-generation solar cells are more effective and efficient, and also, they do not rely on p-n junction design like previous generations did. Perovskites are a class of materials with a distinctive crystal structure called after the mineral that contains it when used to create solar cells, they have showed promise for high performance and low production costs.

II. Analysis of Cu_2O and C_UI as HTL in a Perovskite ($CH_3NH_3PbX_3$, X: I, Br, Cl) Solar Cells

Effect study of Cu_2O in Perovskite Solar Cells as Hole Transport Layer:

The active layer is made of perovskite materials $CH_3NH_3PbX_3$(X:I, Br, Cl), while the HTL is made of Cu_2O for metal back contact. Cu_2O serves as the HTL in perovskite solar cells, allowing the cell's efficiency to be maximized. Figure1 shows the basic structure of the perovskite solar device with ($CH_3NH_3PbX_3$,X: I, Br, Cl) (0.35, 0.40, 0.28 μm).
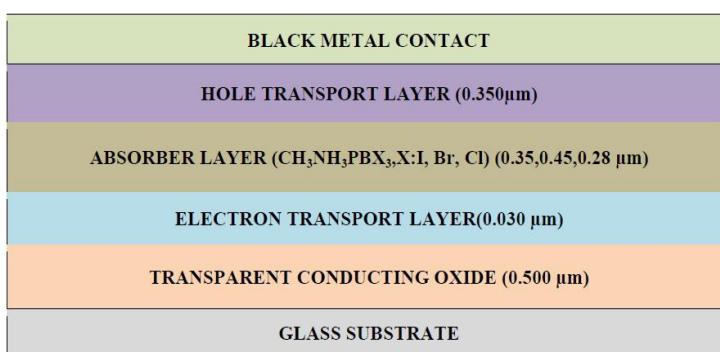

Figure 1: Basic Structure of Perovskite Solar Device with ($CH_3NH_3PbX_3$, X: I, Br, Cl) (0.35, 0.40, 0.28μm)

The SCAPS for several layers of perovskite solar cells, such as TCO, ETL, Absorber ($CH_3NH_3PbI_3$, $CH_3NH_3PbBr_3$, $CH_3NH_3PbCl_3$), and HTL is being utilized for simulation.

Table no 1: SCAPS Simulation parameter of PSCs [1] [2] [3]

Parameter	TCO	ETL	Absorber ($CH_3NH_3PbI_3$)	Absorber ($CH_3NH_3PbBr_3$)	Absorber ($CH_3NH_3PbCl_3$)	HTL (Cu_2O)
Thickness (μm)	0.50	0.030	0.35	0.45	0.28	0.350
Band gap (eV)	3.5	3.2	1.5	2.33	3.1	2.1
Electron affinity (eV)	4	4.26	3.9	3.7	4	3.2
Relative permittivity	9	38	10	10	6.5	7.1
Conduction band density (cm^{-3})	2.00×10^{18}	2.00×10^{18}	2.75×10^{18}	1.00×10^{17}	1.00×10^{19}	2.250×10^{19}
Valance band density (cm^{-3})	1.80×10^{19}	1.80×10^{19}	3.90×10^{18}	1.00×10^{18}	1.00×10^{19}	1.80×10^{19}
Electron mobility ($cm^2 V^{-1} s^{-1}$)	20	4	2	2	50	2.2
Hole mobility ($cm^2 V^{-1} s^{-1}$)	8	2	2	2	50	2.2
Donor concentration (cm^{-3})	2.00×10^{19}	1.00×10^{16}	0	0	1.00×10^{17}	0
Acceptor concentration (cm^{-3})	0	0	2.00×10^{17}	1.00×10^{21}	1.00×10^{17}	1.00×10^{18}
Defect density (cm^{-3})	1.00×10^{15}	1.00×10^{15}	4.5×10^{17}	N/A	N/A	N/A
Capture cross section for electrons (cm^2)	2.00×10^{-15}	1.00×10^{-15}	2.00×10^{-14}	1.00×10^{-14}	1.00×10^{-15}	1.00×10^{-13}
Capture cross section for holes (cm^2)	2.00×10^{-15}	1.00×10^{-15}	2.00×10^{-14}	1.00×10^{-14}	1.00×10^{-15}	1.00×10^{-13}

Impact analysis of Different Active Layer ($CH_3NH_3PbI_3$) Thicknesses In Perovskite Solar Cells using Cu₂O as HTL :

A perovskite solar cell is a "hybrid organic-inorganic lead halide" based cell with a compound perovskite structure that is particularly good in "light-harvesting" of sunlight due to its high "absorption coefficient (cm^{-1})". With the use of the SCAPS tool, numerical simulation, and comprehensive modelling on perovskite solar cells employing perovskite material such as methyl ammonium lead Iodide (MAPbI₃, MA=CH₃NH₃) at various thicknesses were performed.

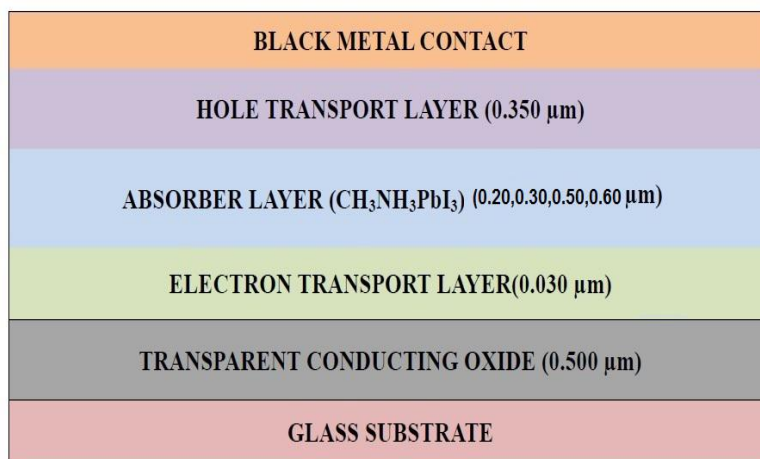Figure 2: Structure of Perovskite Solar Device with Different Thickness 0f Active Layer

For various parameters such as open-circuit voltage (Voc), fill factor (FF), PCE, and short-circuit current density (Jsc), the electrical properties of the MAPbI$_3$ material utilized as active layer have been computed. Figure 2 illustrates the creation of a perovskite solar cell. The HTL is made of cuprous oxide (Cu_2O).

Table no2: Simulation parameters of PSCs using SCAPS [4] [5]

Parameters	TCO	ETL	Absorber ($CH_3NH_3PbI_3$)At 0.20, 0.30, 0.50, 0.60	Cu_2O (HTL)
Thickness (μm)	0.50	0.030	0.35	0.350
Band gap (eV)	3.5	3.2	1.5	2.1
Electron affinity (eV)	4	4.26	3.9	3.2
Relative permittivity	9	38	10	7.1
Conduction band density cm^{-3}	2×10^{18}	2×10^{18}	2.75×10^{18}	2.25×10^{19}
Valance band density cm^{-3}	1.80×10^{19}	1.80×10^{19}	3.90×10^{18}	1.80×10^{19}
Electron mobility($cm^2 V^{-1} s^{-1}$)	20	4	2	2.2
Hole mobility ($cm^2 V^{-1} s^{-1}$)	8	2	2	2.2
Donor concentration cm^{-3}	2×10^{19}	1×10^{16}	0	0
Acceptor concentration cm^{-3}	0	0	2.10×10^{17}	1×10^{18}
Defect density cm^{-3}	1×10^{15}		4.50×10^{17}	N/A
Capture cross section for electrons cm^2	2×10^{-15}	1×10^{-15}	2×10^{-14}	1×10^{-13}
Capture cross section for holes cm^2	2×10^{-15}	1×10^{-15}	2×10^{-14}	1×10^{-13}

Performance Analysis of Cu_2O Perovskite (CH3NH3PbI3) Solar Cell using Different Absorption Coefficient:
The influence of absorption coefficient with cuprous oxide (Cu_2O) as an HTL in perovskite solar cell $CH_3NH_3PbI_3$ was investigated in this study. Figure3 depicts a model of a perovskite solar cell with various 10^3, 10^4, 10^5, and 10^6 absorption coefficients.

Figure 3: Perovskite Solar Device Model with Different Absorption Coefficient of (cm^{-1})

Analysis of CuI as HTL in a Perovskite (CH$_3$NH$_3$PbX$_3$, X: I, Br, Cl) Solar Cell :
In perovskite solar cells, a CuI substance serves as an HTL that improves efficiency. Spiro-MeOTAD has a two-order-of-magnitude lower electrical conductivity than CuI and allows for a substantially higher FF as demonstrated by impedance spectroscopy SCAPS software was used to simulate the entire simulation process for a lead-based perovskite solar cell (CH$_3$NH$_3$PbX$_3$, X: I, Br, Cl) employing TiO$_2$ as the ETL and CuI as the

HTL in the research.

Figure 4: CuI in Perovskite Solar Cell as Hole Transport Layer

Effect Study of CuI in Perovskitesolar Cell as HTL:
To improve efficiency, a perovskite cell structure (CH$_3$NH$_3$PbI$_3$, CH$_3$NH$_3$PbBr$_3$, CH$_3$NH$_3$PbCl$_3$) was adjusted, and several performance parameters such as Jsc, FF, Voc, and PCE were calculated and compared.

Table no 3: Simulation parameters of PSCs devices

Parameters	TCO	ETM (TiO$_2$)	Absorber(CH$_3$NH$_3$PbI$_3$)	HTM (CuI)
Thickness (μm)	0.5	0.030	0.350	0.100
Band gap energy Eg (eV)	3.5	3.2	1.5	2.98
Electron affinity (eV)	4	4.26	3.9	2.1
Relative permittivity e_r	9	3.8×10^8	10	6.5
Effective conduction band density Nccm^{-3}	2×10^{18}	2×10^{18}	2.75×10^{18}	2.8×10^{19}
Effective valance band density Nvcm^{-3}	1.8×10^{19}	1.8×10^{19}	3.9×10^{18}	1×10^{19}
Electron mobility ($cm^2 V^{-1} s^{-1}$)	20	4	10	1.69×10^{-4}
Hole mobility($cm^2 V^{-1} s^{-1}$)	8	2	10	1.69×10^{-4}
Donor concentration NDcm^{-3}	2×10^{19}	1×10^{16}	0	0
Acceptor concentration NA cm^{-3}	0	0	2.1×10^{17}	1×10^{18}
Defect density Ntcm^{-3}	1×10^{15}	1×10^{15}	4.5×10^{17}	1×10^{15}

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III. Results and Discussion

The Different Results of Perovskite (CH$_3$NH$_3$PbX$_3$, X: I,Br, Cl) Solar Cell using Cu$_2$O as HTL:

When compared to other perovskite materials, the CH$_3$NH$_3$PbI$_3$ perovskite solar cell has a better open circuit voltage (Voc) =0.715, short circuit current density (Jsc)=25.573, fill factor (FF) =77.05, and PCE =16.65. Also, the various parameters of perovskite solar cells using CH$_3$NH$_3$PbBr$_3$ are Voc =0.774, Jsc =6.931, FF =78.52, and PCE =5.21 for CH$_3$NH$_3$PbBr$_3$, and Voc =0.758, Jsc =1.068, FF =74.52, and PCE =0.73 for CH$_3$NH$_3$PbCl$_3$ for perovskite solar cells using CH$_3$NH$_3$Pb. Table 4 shows the various simulated parameters for perovskite (CH$_3$NH$_3$PbI$_3$)solar cell using different 0.20, 0.30 and 0.50 and 0.60 thickness. Table 3.4 shows different simulated parameters for CH$_3$NH$_3$PbI$_3$ perovskite solar cell with various absorption coefficients (cm-1) like 103, 104, 105, 106. The various absorption coefficients such as 10^3, 10^4, 10^5, 10^6 on the perovskite cell CH$_3$NH$_3$PbI$_3$ have been modified and calculated the different performance parameters such as Jsc, FF,Voc, PCE, C-F, and C-V. The simulation is done under dark and light illumination conditions. In the dark illumination condition, the working point voltage is zero. In the light illumination condition, the simulation is done at a working point voltage is 0.5V for all perovskite solar cell materials.

Table no 4: The Various simulated parameters for perovskite (CH$_3$NH$_3$PbI$_3$) solar cell using different 0.20 (μm), 0.30 (μm) and 0.50(μm) and 0.60(μm) thickness.

ThicknessofPerovskite(CH3NH3PbI3)Material(μm)	PARAMETER			
	Voc (V)	Jsc (mAcm-2)	FF	PCE (%)
At 0.20 (μm)	0.76	24.18	90.10	14.64
At 0.30 (μm)	0.75	24.19	91.75	14.98
At 0.50 (μm)	0.73	24.20	94.27	15.29
At 0.60 (μm)	0.715	25.573	98.23	16.65

Table no 5: Different simulated parameters for $CH_3NH_3PbI_3$ perovskite solar cell with various 10^3, 10^4, 10^5, 10^6 absorption coefficients (cm-1).

Absorption Coefficient of cm^{-1}	PARAMETER			
	Voc (V)	Jsc (mAcm-2)	FF	PCE (%)
10^3	0.7103	24.40	95.01	15.22
10^4	0.7833	25.01	96.32	15.73
10^5	0.8227	25.93	97.98	16.65
10^6	0.8992	27.33	98.47	16.88

J-V Characteristics for the $CH_3NH_3PbI_3$ Perovskite Solar Cell:

The J-V characteristic of perovskite solar cells with a perovskite active layer like $CH_3NH_3PbI_3$ has been displayed. When compared to other perovskite materials, the Voc=0.715, Jsc=25.573, FF=77.05, and PCE=16.65 characteristics of the $CH_3NH_3PbI_3$ perovskite solar cell are better. The J-V characteristics of the investigated perovskite solar cell have been shown, and the cell parameters have been extracted in Figure 4.
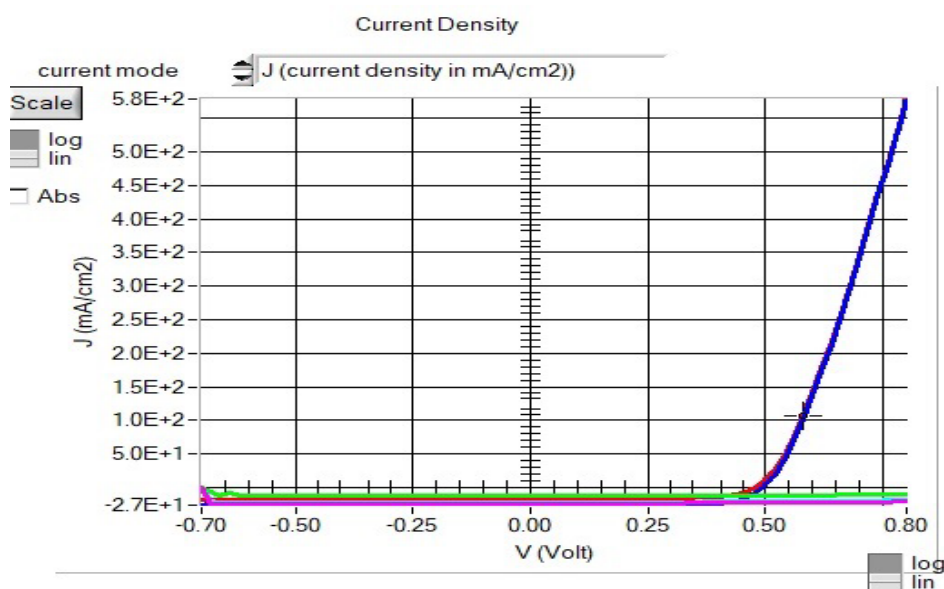
Figure 5: J-V Characteristics for the $CH_3NH_3PbI_3$ Perovskite Solar Cell

The J-V characteristic of perovskite solar cells with a perovskite active layer like $CH_3NH_3PbI_3$ has been displayed. When compared to other perovskite materials, the Voc=0.715, Jsc=25.573, FF=77.05, and PCE=16.65 characteristics of the $CH_3NH_3PbI_3$ perovskite solar cell are better. The J-V characteristics of the investigated perovskite solar cell have been shown, and the cell parameters have been extracted in Figure 5.

Quantum Efficiency (QE) Characteristic for $CH_3NH_3PbI_3$ Perovskite Solar Cell:

The quantum efficiency (QE) characteristics have been plotted for the perovskite solar cell $CH_3NH_3PbI_3$ at the absorption coefficient of 10^5 (cm^{-1}) shown in Figure 6.
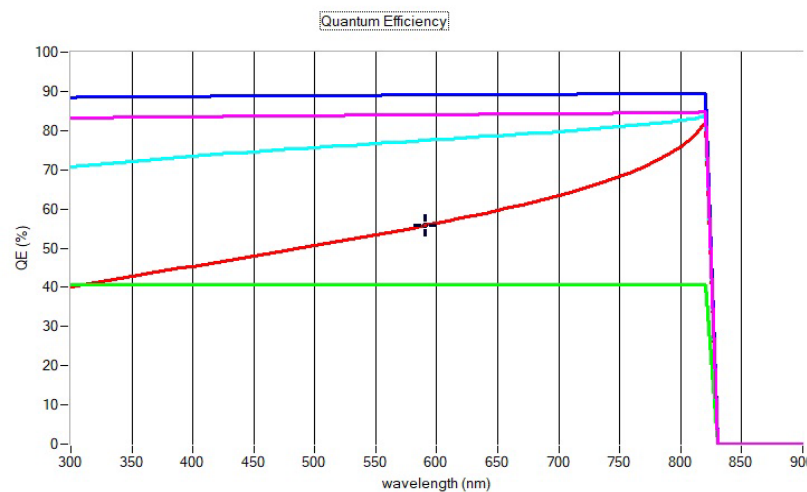
Figure 6: Quantum Efficiency (QE) Characteristic for $CH_3NH_3PbI_3$ Perovskite Solar Cell

Final Result of Simulation on SCAPS Using: Fig.7 depicts the simulation's ultimate outcome, which includes all parameters such as open-circuit voltage (Voc) =0.945, short-circuit current density (Jsc)=24.190, FF=77.99, and
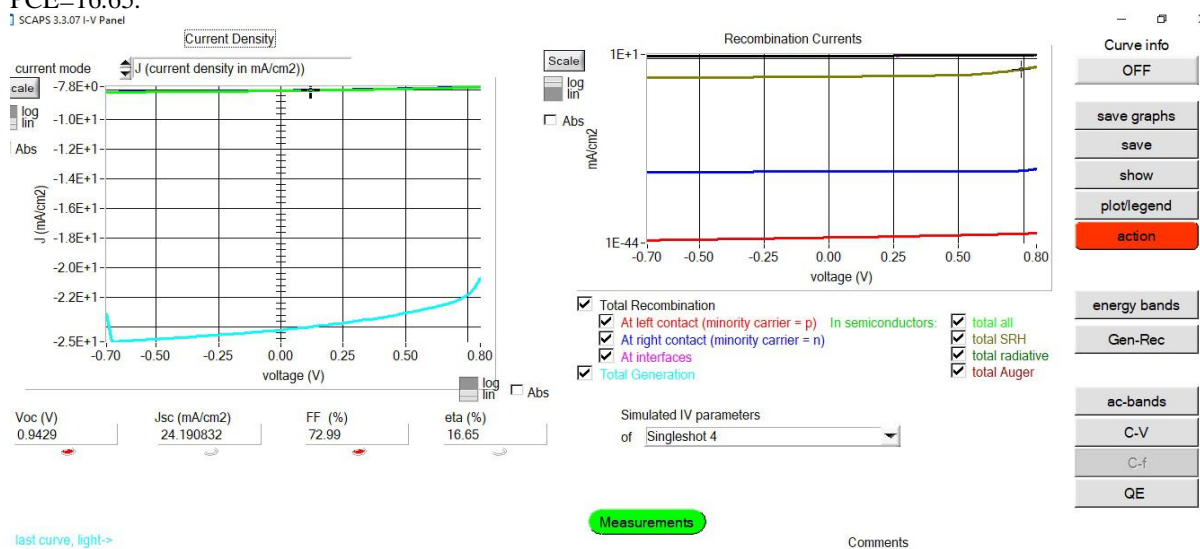PCE=16.65.

Figure7: Final Result of Simulation on SCAPS

Table no 6: Comparison between previous work [1] and work performed in this study.

MATERIAL		PARAMETER			
		Voc (V)	Jsc (mAcm-2)	FF	PCE (%)
CH3NH3PbI3	Reported [1]	0.61	15.57	71.69	6.85
	Present Work	0.9429	24.190	72.99	16.65
CH3NH3PbBr3		1.90	7.65	76.36	11.43
CH3NH3PbCl3		1.68	1.18	73.40	1.46

Table no 7: Optimized parameters of the device.

Optimized parameters	ETM (TiO₂)	Absorber (CH₃NH₃PbI₃)	HTM (CuI)
Doping density cm^{-3}	N/A	5×10^{16}	5×10^{19}
Electron affnity (eV)	3.85	N/A	2.57
Defect density cm^{-3}	N/A	1×10^{15}	N/A
Thickness (nm)	N/A	600	N/A
Hole mobility $cm^2 V^{-1} s^{-1}$	N/A	N/A	5×10^{-2}

The Different Results of Perovskite (CH3NH3PbX3,X: I, Br, Cl) Solar Cell using CUI as HTL:
Table 8 shows the comparison between previous work and work performed in this paper.

Table no 8: Photovoltaic parameters of CuI based perovskite solar cells reported in the experimental work in the literature and simulated results using SCAPS.

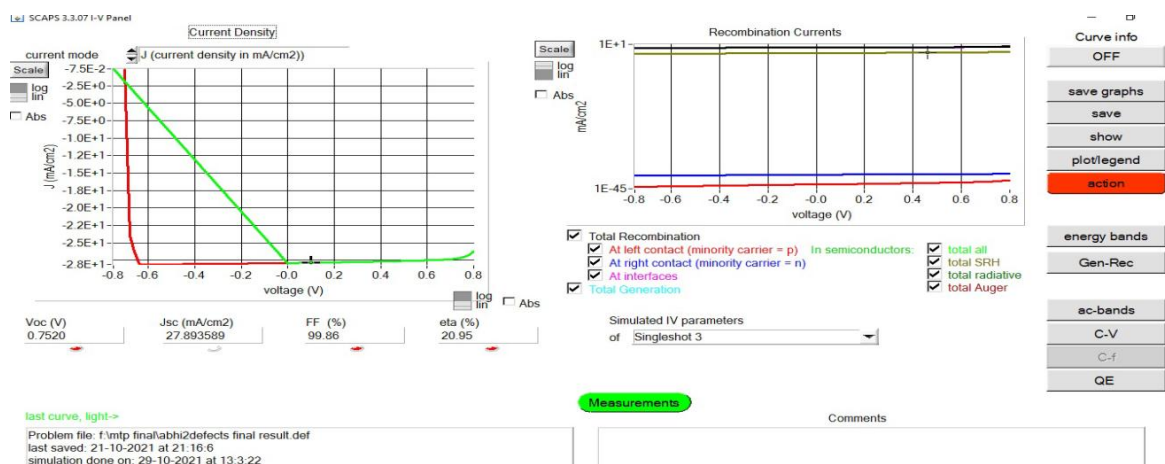| Parameters	Initial	Optimized NA of Absorber	Optimized ETM	Optimized Nt and thickness	Optimized (μm) and NA of HTM	Final	[6]	[7]	[8]
PCE (%)	6.85	8.31	10.28	10.80	6.92	20.95	17.60	6	7.5
FF (%)	71.69	68.97	69.85	78.65	72.31	99.86	75	62	57
Jsc ($mA cm^2$)	15.57	18.47	16.35	21.92	15.60	27.89	22.78	17.8	16.7
Voc (V)	0.61	0.65	0.90	0.63	0.61	0.75	1.03	0.55	0.78

Figure 8: Final Result of the Simulation

Figure 4.6 shows the final result of the simulation including all the parameters like open-circuit voltage (Voc) =0.7520 short circuit current density (Jsc) =27.89, fill factor (FF)=99.86, and PCE=20.95.

Quantum Efficiency (QE) Characteristic for CH₃NH₃PbI₃ Perovskite Solar Cell:

The quantum efficiency (QE) characteristics have been plotted for the perovskite solar cell CH3NH3PbI3 at the absorption coefficient of 105 (cm^{-1}) shown in Figure 9.
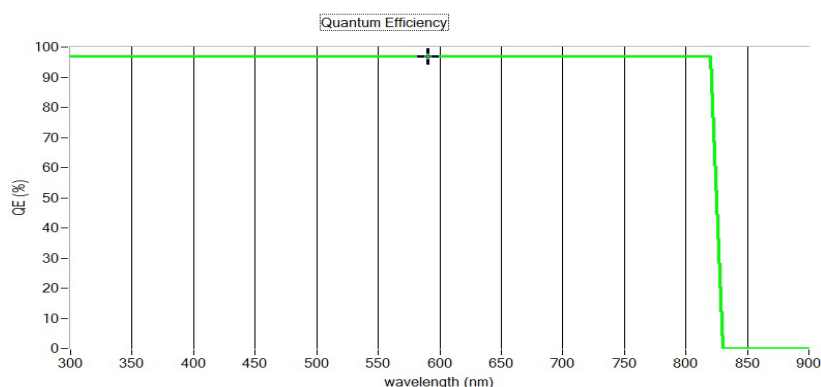

Figure 9: Quantum Efficiency (QE) characteristic for CH$_3$NH$_3$PbI$_3$ Perovskite Solar Cell

The J-V Characteristics for the CH$_3$NH$_3$PbI$_3$ Perovskite Solar Cell:

The J-V characteristic of perovskite solar cells with a perovskite active layer like CH3NH3PbI3 has been displayed. When compared to other perovskite materials, the Voc=0.7520, Jsc=27.89, FF=99.86, and PCE=20.95 characteristics of the CH$_3$NH$_3$PbI$_3$ perovskite solar cell are better.
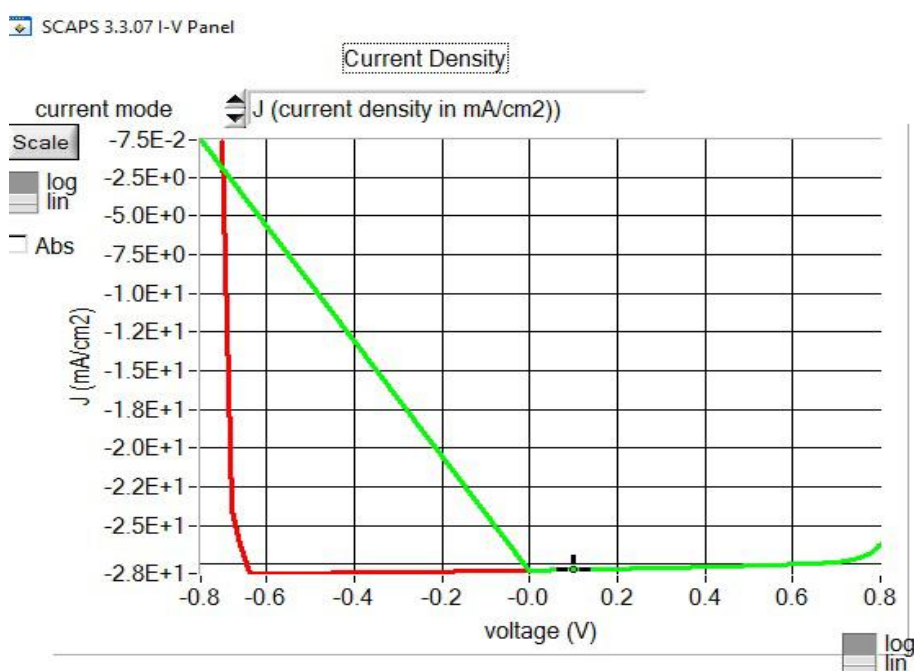

Figure10: J-V Characteristics of CH$_3$NH$_3$PbI$_3$ Perovskite Solar Cell

IV. Conclusion

This paper presents the research work conducted on perovskite solar cells for various HTL materials and absorption materials (CH$_3$NH$_3$PbX$_3$, X: I, Br, Cl). Perovskite cells are the future of solar cells. The PCE of solar cells is an open area for research and various works are already done in this area. The primary objective of most of the research works is to improve PCE while satisfying other parameters like Voc, Jsc, and FF. The PCE depends on various factors like the thickness of the absorber, absorber coefficient, and doping levels. The HTL materials play a vital role in determining the PCE of perovskite cells. In this price-oriented market, the price of solar cells is also dependent on these HTL materials. In this research work, authors have analysed the performance of solar cells for various HTL materials and enhanced the PCE of solar cells considering the thickness of the absorber as a parameter. Our results conclude that the PCE of solar cells is 16.65 which is much

better than the previous research works where PCE values were about 6.85% to 9.23%. Our work improves the PCE. A detailed analysis is shown for the performance of solar cells concerning variation in absorber coefficient and thickness. The results conclude that the PCE of solar cell is 20.95%. In the future, other HTL materials can be used. Few research works are already conducted for HTL materials n-ZnSe; p-MASnI3; p-CuSCN, etc. These materials will play a vital role in the future to improve the performance of the solar cell.

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