

**OPTIMIZING THE EFFICIENCY OF  
PEROVSKITE SOLAR CELL BY INCREASING  
THICKNESS AND TEMPERATURE**



**ZAINAB FATIMA**

**DEPARTMENT OF PHYSICS  
KINNAIRD COLLEGE FOR WOMEN,  
LAHORE, PAKISTAN  
2023.**

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SOLAR CELL BY INCREASING THICKNESS AND  
TEMPERATURE**



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IN  
PHYSICS**

**By  
ZAINAB FATIMA**

**DEPARTMENT OF PHYSICS  
KINNAIRD COLLEGE FOR WOMEN, LAHORE  
2023.**

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**Supervisor:**

Dated: 17-05-2023

\_\_\_\_\_

**Saima Mubeen**

Assistant Professor in Physics

Kinnaird College for Women, Lahore.

\_\_\_\_\_

**Ayesha Aftab**

Head of the Department

Kinnaird College for Women, Lahore.

“All changes suggested by examiners during defense are incorporated in this final copy.”

\_\_\_\_\_

Student

\_\_\_\_\_

Supervisor

\_\_\_\_\_

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**Zainab Fatima**

Registration No: F19BPHY001

Program: BS PHYSICS

Signature:



**Supervisor:**

---

**Saima Mubeen**

Assistant Professor in Physics

Kinnaird College for Women, Lahore.

---

**Ayesha Aftab**

Head of the Department

Kinnaird College for Women, Lahore.

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Zainab Fatima

## ABSTRACT

The development of photovoltaic technologies have sparked significantly in last three decades. The major factor being low cost, more reliability and high efficiency. The simulation techniques used to minimize the size of devices are such as solar cells and to reduce the time for research period. Solar cells are the promising renewable resource that uses tri-valent and penta-valent compounds to achieve energy conversions. In this study the most extensively investigated perovskite methy-ammonium lead iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) is used as an active absorber layer and the impact of thickness and temperature on their performances will be the main parameters to be studied. In this paper, SCAPS-1D will be used for the simulation process in order to study the parameters such as open-circuit voltage ( $V_{oc}$ ), short-circuit current ( $J_{sc}$ ), Fill Factor (FF) % and Efficiency. This will be done by varying the thickness and temperature. The thickness is being varied from 100nm to 700nm and temperature will be varied from 300K-500K. As the thickness of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  increases, decrease in open circuit voltage  $V_{oc}$ , increase in the short circuit current  $J_{sc}$  will be observed. Also the increase of the efficiency and decrease of the Fill Factor (FF) will also be observed. Similarly, when the temperature is being varied by keeping the thickness constant for 700nm change in the parametric values will also be observed. As the temperature is increased there is a sudden drop in the efficiency of the solar cell. Also the short circuit current ( $J_{sc}$ ), open circuit voltage ( $V_{oc}$ ) and Fill Factor (FF) decreased.

# **OPTIMIZING THE EFFICIENCY OF PEROVSKITE SOLAR CELL BY INCREASING THICKNESS AND TEMPERATURE**

## **TABLE OF CONTENTS**

<b>Chapter</b>	<b>Title</b>	<b>Page</b>
	<b>RESEARCH COMPLETION CERTIFICATE</b>	<b>ii</b>
	<b>ANTI-PLAGIARISM DECLARATION</b>	<b>iii</b>
	<b>ACKNOWLEDGEMENT</b>	<b>iv</b>
	<b>ABSTRACT</b>	<b>v</b>
	<b>TABLE OF CONTENTS</b>	<b>vi</b>
	<b>LIST OF FIGURES</b>	<b>vi</b>
	<b>LIST OF TABLES</b>	<b>vi</b>
	<b>LIST OF ABBREVIATIONS</b>	<b>vi</b>
<b>1</b>	<b>INTRODUCTION</b>	<b>1</b>
	1.1 Solar cell	1
	1.2 History of Solar Cell	1
	1.3 Physics of Solar Cell	1
	1.4 Light absorption	2
	1.5 Electron-hole pair production	3
	1.6 Transport of electron and hole towards electrode	4
	1.7 Generation of Solar Cell	4
	1.7.1 First Generation	6
	1.7.2 Second Generation	6
	1.7.3 Third Generation	6

1.7.4 Fourth Generation	6
1.8 Solar Cell Design	7
1.8.1 Homo-junction Solar Cell	7
1.8.2 Hetero-junction Solar Cell	8
1.9 Paramters	10
1.9.1 Open circuit voltage (Voc)	10
1.9.2 Short circuit voltage (Jsc)	11
1.9.3 Fill Factor (FF)	12
1.9.4 Efficiency	12
1.10 Perovskite Solar Cell (PSC)	13
1.10.1 ETL (Electron Transport Layer)	14
1.10.2 HTL (Hole Transport Layer)	14
1.10.3 Absorber Layer	15
1.10.4 Electrodes	16
1.11 Material of Solar Cell (CH <sub>3</sub> NH <sub>3</sub> PBI <sub>3</sub> )	17
<b>RATIONALE</b>	<b>19</b>
<b>OBJECTIVE OF THE STUDY</b>	<b>20</b>
<b>2 LITERATURE REVIEW</b>	<b>21</b>
<b>3 MATERIALS AND METHODS</b>	<b>26</b>
3.1 SCAPS	26
3.2 Characteristics of SCAPS	26
3.3 Getting started with SCAPS	26
3.3.1 Basics of SCAPS	26
3.3.2 Run SCAPS	27
3.3.3 Define the Problem	27
3.3.4 Define the Working Point	27

3.3.5 Select the measurements to stimulate	<b>28</b>
3.3.6 Start the Calculations	<b>28</b>
3.3.7 Display the stimulated curves	<b>29</b>
3.3.8 Editing the Problem	<b>29</b>
3.4 Solar cell definition	<b>29</b>
3.4.1 Editing a solar cell definition	<b>29</b>
3.4.2 References convention for the voltage and current	<b>30</b>
3.4.3 Contacts	<b>31</b>
3.4.4 Layer Thickness	<b>31</b>
3.4.5 The constant layer of an optical absorption	<b>31</b>
3.4.6 A material Approach	<b>32</b>
3.4.6.1 Saving materials	<b>32</b>
3.4.6.2 Loading material	<b>32</b>
3.5 Illumination conditions	<b>32</b>
3.6 Internal SCAPS calculation	<b>32</b>
3.7 The generation models	<b>32</b>
3.7.1 Constant generation G	<b>32</b>
3.8 Shunt conductance and series resistance	<b>33</b>
3.9 Navigating to the analysis	<b>33</b>
3.10 Curve info and legend	<b>33</b>
3.11 I-V panel	<b>33</b>
3.12 Introduction to Origin	<b>34</b>
3.13 Characteristics of Origin	<b>34</b>
3.14 Getting started with origin	<b>34</b>
3.14.1 The basics	<b>34</b>

3.14.2	Run Origin	35
3.14.3	Define the Paramters	35
3.14.4	Setting the values and columns	36
3.14.5	Start plotting	37
3.15	Graph Interface	37
3.15.1	Editing the axis	38
3.15.2	Saving the graph	39
<b>4</b>	<b>RESULTS AND DISCUSSION</b>	<b>40</b>
4.1	CH <sub>3</sub> NH <sub>3</sub> PBI <sub>3</sub>	40
4.2	Effect of thickness	42
4.2.1	Effect of thickness on open circuit voltage (Voc)	43
4.2.2	Effect of thickness on current density (Jsc)	43
4.2.3	Effect of thickness on Fill Factor (FF)	44
4.2.4	Effect of thickness on efficiency	46
4.3	Effect of temperature	47
4.3.1	Effect of temperature on open circuit voltage (Voc)	47
4.3.2	Effect of temperature on short circuit voltage (Jsc)	48
4.3.3	Effect of temperature on Fill Factor (FF)	49
4.3.4	Effect of temperature on efficiency	50
	<b>CONCLUSION</b>	<b>52</b>
	<b>LIMITATIONS</b>	<b>53</b>
	<b>RECOMMENDATIONS</b>	<b>54</b>
	<b>REFERENCES</b>	<b>55</b>
	<b>TURNITIN REPORT</b>	



# LIST OF FIGURES

<b>Figure</b>	<b>Title</b>	<b>Page</b>
1.1	Light Absorption	2
1.2	Light Absorption phenomenon	2
1.3	Molecular Orbitals of Solar Cell	3
1.4	Electron-hole pair generation	4
1.5	Three generation of cell	5
1.6	Fourth-generation of cell	5
1.7	Homo-junction perovskite cell	77
1.8	Homo-junction perovskite solar cell	9
1.9	Hetero-junction solar cell	9
1.10	Hetero-junction perovskite solar cell	10
1.11	Open circuit voltage for IV-curve	11
1.12	Short circuit voltage for IV-curve	12
1.13	Fill Factor (FF) for IV-curve	12
1.14	Efficiency for IV-curve	13
1.15	Perovskite solar cell crystal molecular and multilayers structure	14
1.16	Perovskite solar cell structure	14
1.17	Electron transport layer in perovskite solar cell	15
1.18	Hole transport layer in Perovskite Solar cell	16
3.1	Action Panel of SCAPS	27
3.2	Action Panel of SCAPS	28
3.3	Stimulated curves in SCAPS	29
3.4	Solar cell definition	30
3.5	Numerical setting panel	30
3.6	Left contact in solar cell definition panel	31
3.7	Panel of shunt conductance and series resistance	33
3.8	I-V Panel	34

3.9	Workbook interface in Origin	35
3.10	Defining the parameter	36
3.11	Setting values in column	36
3.12	Plotting panel	37
3.13	Graph interface	37
3.14	Axis action pane	38
3.15	Exporting graph	38
3.16	Selecting type for exporting graph	39
4.1	Schematic structure of $\text{CH}_3\text{NH}_3\text{PbI}_3$	40

## LIST OF TABLE

<b>Table</b>	<b>Title</b>	<b>Page</b>
4.1	Parameter of CH <sub>3</sub> NH <sub>3</sub> PBI <sub>3</sub>	
4.2	Parameters of Spiro-OMeTAD and FTO	
4.3	Values of Voc with increase of thickness	
4.4	Values of Jsc with increase of thickness	
4.5	Values of FF (fill factor) with increase of thickness	
4.6	Effect of thickness increase on the Efficiency	
4.7	Effect of temperature on open circuit voltage (Voc)	
4.8	Effect of temperature on short circuit voltage (Jsc)	
4.9	Effect of temperature on the FF%	
4.10	Effect on Efficiency with the increase of the temperature	

## LIST OF ABBREVIATIONS

SC	Solar Cell
$\text{CH}_3\text{NH}_3\text{PbI}_3$	Methyl Ammonium lead iodide
PSC	Perovskite Solar Cell
PV	Photovoltaic
SCAPS	Solar Cell Capacitance Simulator
FF	Fill Factor
$V_{oc}$	Open circuit voltage
$J_{sc}$	Short circuit current
HTL	Hole Transport Layer
ETL	Electron Transport Layer

# CHAPTER 1

## INTRODUCTION

### 1.1 Solar Cell

Solar cells or photovoltaic (PV) cells are non-mechanical devices that use sunshine to generate energy. Some PV cells can generate electricity from artificial light. Photovoltaic energy conversion involves number of materials and methods. They are made up of semiconductor materials that are basically in the form of a p-n junction [1].

### 1.2 History of Solar Cell

A mechanism was being discovered that named as the photovoltaic effect. In this process, an electric current or voltage generates when exposed to light or other radiant radiation, in 1839. The first solar cell was developed by a Russian scientist by the name of Aleksandr Stoletov using the photoelectric effect, or when light strikes a substance and electrons are liberated. [2].

### 1.3 Physics of Solar cell

P-type and n-type silicon are two different types of semiconductors that are used to make solar cells. Atoms with one fewer electron in their outer energy level than silicon, such boron or gallium, are added to create p-type silicon. An electron vacancy or "hole" is produced in boron because it has one fewer electron than is necessary to make the bonds with the neighbouring silicon atoms. By adding elements, like phosphorus, that have one extra electron in their outer level than silicon, the n-type silicon is created. The outer energy level of phosphorus contains five electrons, not four. It forms bonds with the silicon atoms next to it, however the bonds do not include one electron. It may instead move around freely inside the silicon framework [3], [4].

### 1.4 Light absorption

The absorption coefficient is being determined by the absorption intensity of the light from the sun. The reason why blue light has a high absorption coefficient

and is absorbed at a close proximity to the surface (a few microns for silicon solar cells) is shown by this fact. Red light, on the other hand, is absorbed less forcefully because of its lower energy and longer wavelength. When a photon's energy is being equal to or greater than the material's band gap, the material absorbs the photons that is being hitted on it, thus it excite an electron into the lowest unoccupied level [5].

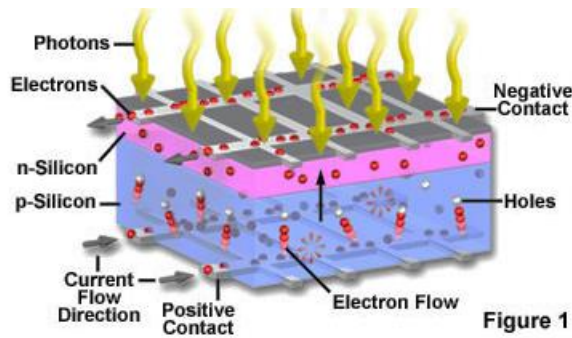


Figure 1.1 Light Absorption [5].

When a photon is being absorbed there created a minority carrier and a majority carrier. The creation of these charge carriers by photons generation is essential for the energy production in basic solar systems [5].

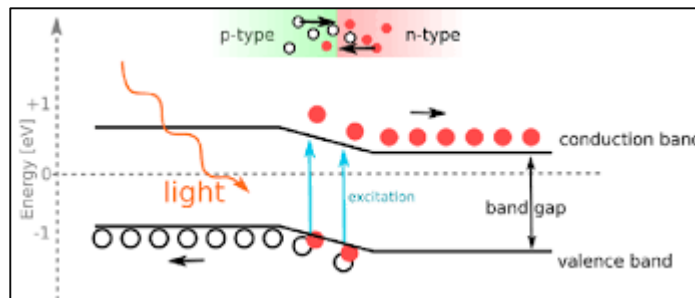


Figure 1.2 Light Absorption Phenomenon [6].

## 1.5 Electron hole pair generation

After the voltage is being applied, the incident photon being almost has an energy that is larger than the band gap. Then the electron-hole pairs will be produced in the solar cell. Just because of their meta-stability, the electrons in p-type materials and the holes in n-type materials can only exist only for about as long as the minority carrier lifetime before recombining. After that, if the carrier recombines, the electron-hole pair from which the light is being produced, there no current or power will be produced [7].

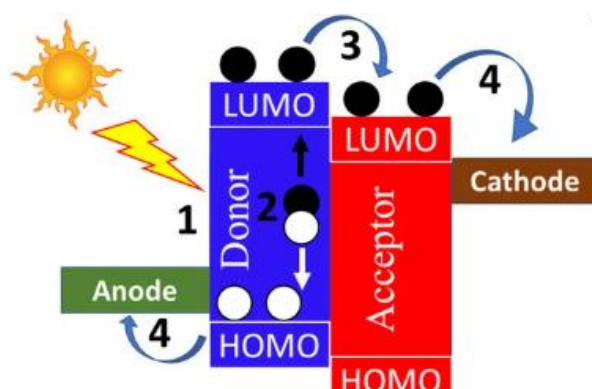


Figure 1.3 Molecular orbitals of solar cell [7].

When the electrons that are being present in the lowest energy band, the valance electrons are vacating a space in the highest occupied molecular orbital. The highest occupied level thus creates a hole when the lowest unoccupied level has just one electron. At the end, an electron-hole pair is created. [7].

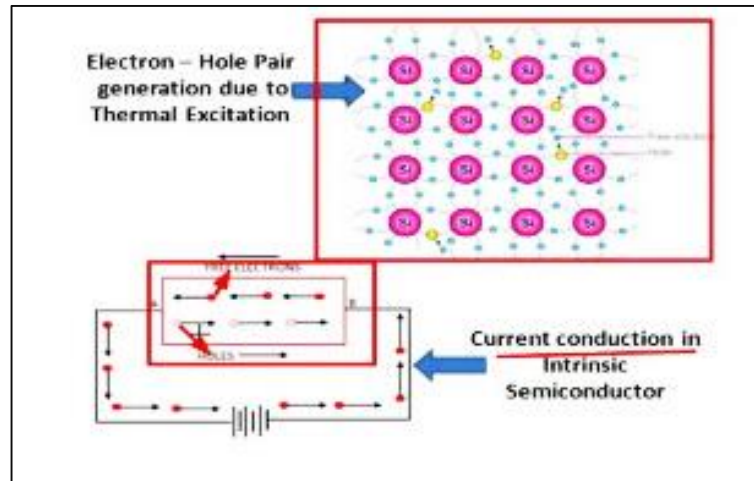


Figure 1.4 Electron-hole pair generation [7].

## 1.6 Transport of electrons and hole towards electrode

The photons that are absorbed produce excitons, which are bonded electron-hole pairs. These excitons diffuse to the perovskite layer's two sides, where they interact with the hole transport layer HTL on one side and the electron transport layer ETL on the other. The excitons' associated holes return to the HTL. While the ETL draws the electrons from the excitons. The same thing occurs when excitons enter the HTL; the HTL draws holes from them, leaving the electrons behind to return to the ETL and be drawn and carried to the cathode. When a voltage source's positive terminal is coupled with the p-type region. Electrons are forward-biased in this situation. This being participates in the creation of covalent bonds in the p-type material. As a result, few covalent connections are broken and electrons are shifted towards the positive terminal [8].

## 1.7 Generation of Solar Cell

The majority of solar cells fall into one of three categories that mainly depends on the light that is being emitted from the sun and thus it is well directed toward the Earth's surface: third-generation solar cells, thin-film solar cells, and crystalline silicon solar cells. [9].

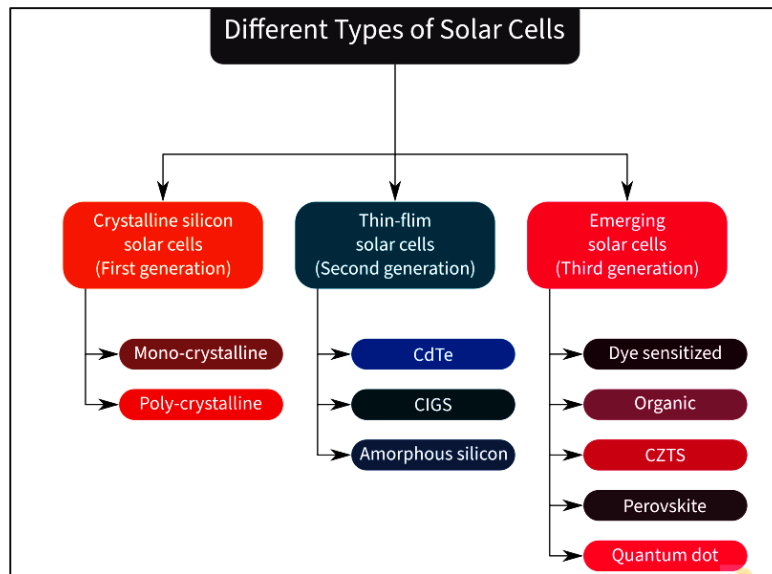


Figure 1.5 Three-generation of solar cell [9].

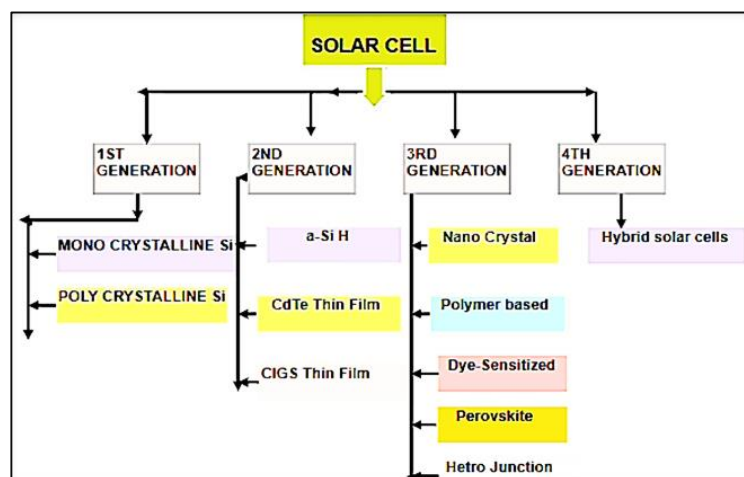


Figure 1.6 Fourth-generation of solar cell [10].

### 1.7.1 First Generation

Crystalline silicon solar cells are first-generation photovoltaic cells. They are made of crystalline silicon (c-Si), also known as silicon crystal. The crystalline solar cells being have great efficiency is the cause. Monocrystalline silicon and polycrystalline silicon are being the two varieties of crystalline silicon [11].

### **1.7.2 Second Generation**

The more recent photovoltaic technology known as thin-film solar cells is made up of one or more thin sheets of photovoltaic materials on a substrate. Flexibility is a benefit. The film's thickness is measured in nanometers. [11].

### **1.7.3 Third Generation**

New solar cell technology is third generation. They are still in a developing condition. Dyesensitized, organic, CZTS, perovskite, and quantum dots are the most well-liked types of them [11].

### **1.7.4 Fourth Generation**

They are basically termed as 4G solar cell technology, also termed as hybrid inorganic solar cells. They are more affordable and have more stability as compared to other generations. They are being having nanoparticle structure, oxides of metal, nano-tubes of the carbon, grapheme and also their derivatives. They are being also referred to as hybrid inorganic cells [11]

## **1.8 Solar Cell Design**

There are mainly two types of design of solar cell:

- Homo-junction solar-cell
- Hetero-junction solar-cell

### **1.8.1 Homo-junction Solar Cell**

In a solar cell made of a single material, the space between an n- and p-layer is known as a homo-junction. In case of homo-junction solar cell the band gap is almost same and the crystalline structure is same. Examples of homo-junction devices are solar cells made of crystalline silicon. Crystalline silicon is modified in a homo-junction cell so that one side is p-type. While the other side is n-type. The p-n junction is positioned so that the greatest quantity of light absorption occurs close to it [12].

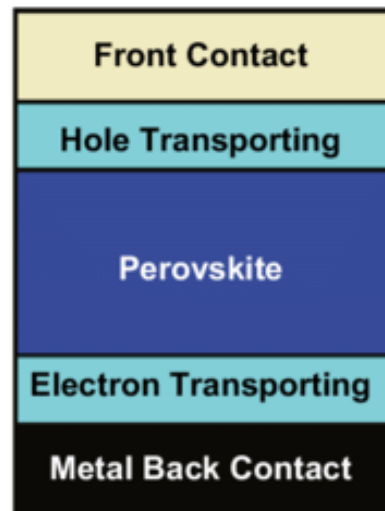


Figure 1.7 Homo-junction Perovskite solar cell [12].

As far we know about the perovskite solar cell they basically have p-i-n structure. The adaptability and transparency of perovskite solar cells can expand their potential applications, improve their operational stability, and lower their production costs [12].

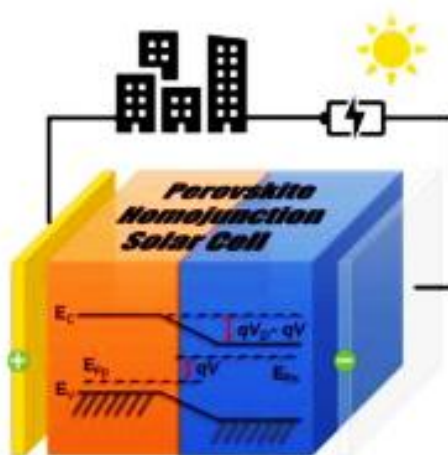


Figure 1.8 3-D Homo-junction Perovskite solar cell [12].

## 1.8.2 Hetero-junction Solar cell

A hetero-junction solar cell is being one of that SC that is basically composed of the two materials separated by contact and their band gaps are not equal. In contrast to conventional silicon solar panels, heterojunction solar cells combine two different materials that are being into one cell: a crystalline silicon cell that is basically being sandwiched between two layers of amorphous "thin-film" silicon. This boosts the efficiency of the panels and makes it easier to harvest more energy [13].

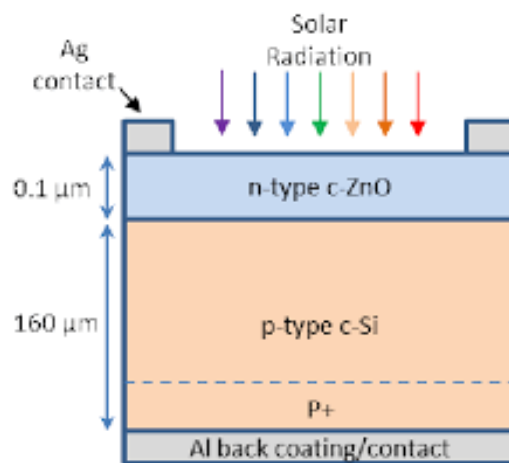


Figure 1.9 Hetero-junction solar cell [13].

The lead based solar cell that has always involved the doping of the ETL and HTL layers is the best sample of the hetero-junction perovskite solar cell as their band-gap is not being equal [13].

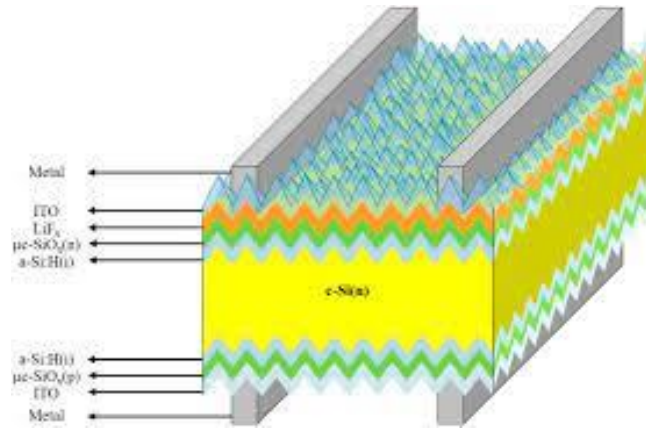


Figure 1.10 Hetero-junction Perovskite solar cell [13].

## 1.9 Parameters

The main parameters are four that are briefly discussed below:

### 1.9.1 Open circuit voltage ( $V_{oc}$ )

The highest voltage a solar cell that is being produced while there is almost no current flowing through it, that why it is being known as the open-circuit voltage ( $V_{oc}$ ). The open-circuit voltage actually reflects the main amount of forward bias on the solar cell that is being caused by the junction's bias only with the current that is being produced by light [13], [14].

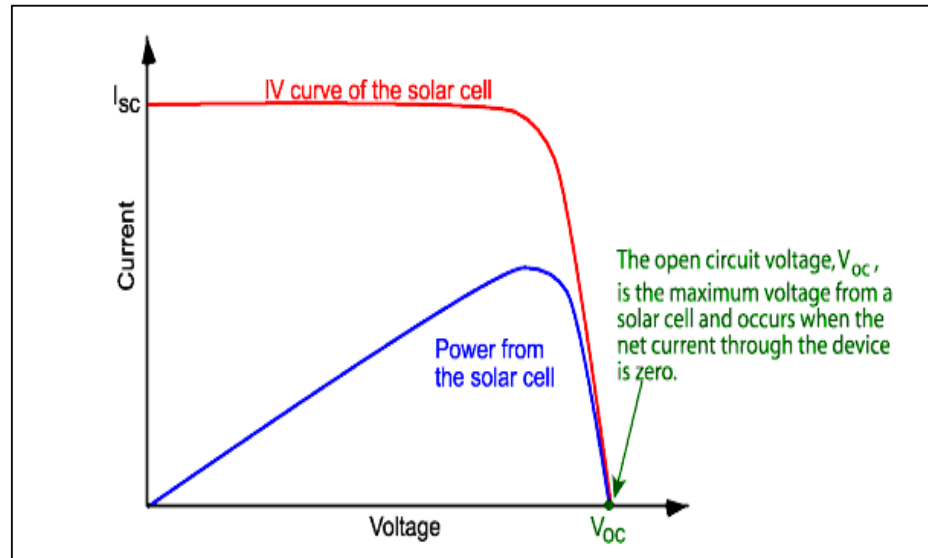


Figure 1.11 Open circuit voltage for IV-curve [13]

The equation for open circuit voltage  $V_{oc}$  of the solar cell is given below;

$$V_{oc} = n_{idL} \frac{k_B T}{q} \ln \left( \frac{J_{ph}}{j_s} + 1 \right)$$

Here we can see that,

- the variable  $n$  is the carrier concentration,
- variable  $q$  is the charge
- $k$  is the Boltzmann constant
- $I_L$  is the light current and  $T$  is the temperature.

### 1.9.2 Short circuit current ( $J_{sc}$ )

The current flowing through the solar cell when the voltage across it is zero, or when the solar cell is shorted out, is known as the short-circuit current. The short-circuit current, which is sometimes abbreviated as ISC,

is seen on the IV curve below. The short-circuit current and the current that produces light are equal for a perfect solar [13].

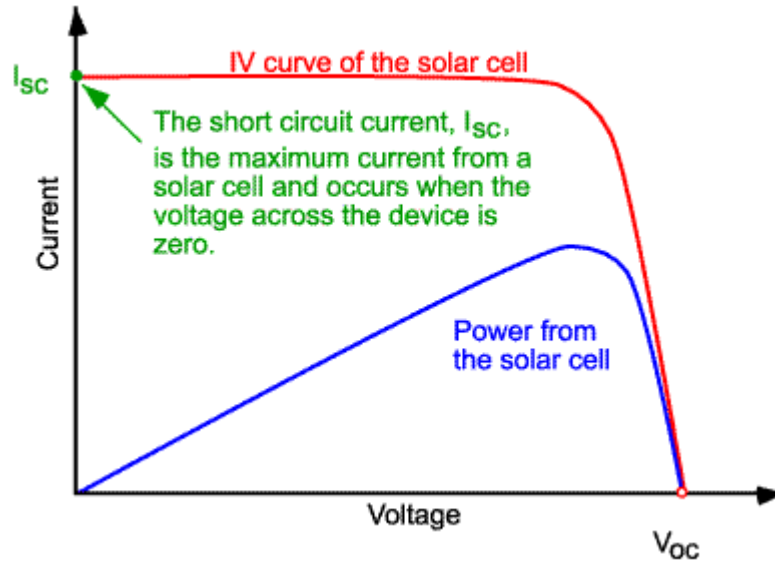


Figure 1.12 Short circuit current for IV-curve

The following list of factors, each of which has an impact on short-circuit current, is provided [13]:

- **The solar cell's surface area:** It is more typical to specify the short-circuit current density ( $J_{sc}$  in  $\text{mA}/\text{cm}^2$ ) rather than the short-circuit current.
- **Effect of Light Intensity:**  $I_{sc}$  from a solar cell is directly correlated with light intensity;
- **The light's colour spectrum at impact:** The spectrum is standardised to the AM1.5 spectrum for the majority of solar cell measurements.
- **The solar cell's optical characteristics (absorption and reflection:** Optical Losses); **a minority carrier** would gather on the

solar cell's surface and in the base, which is mostly dependent on surface passivation and minority carrier lifetime [13].

$$J_{sc} = \int (\lambda)(\lambda)d\lambda \quad (1.2)$$

### 1.9.3 Fill Factor (FF)

The parameter known as "fill factor," more usually abbreviated as "FF," it basically defines the maximum power output along with  $J_{sc}$  and  $V_{oc}$  from a solar cell. The FF is actually being defined as the ratio of the solar cell's maximum power to the sum of  $V_{oc}$  and  $I_{sc}$  [13].

FF is given as follows:

$$FF = \frac{PMP}{V_{oc} \times J_{sc}} \quad (1.3)$$

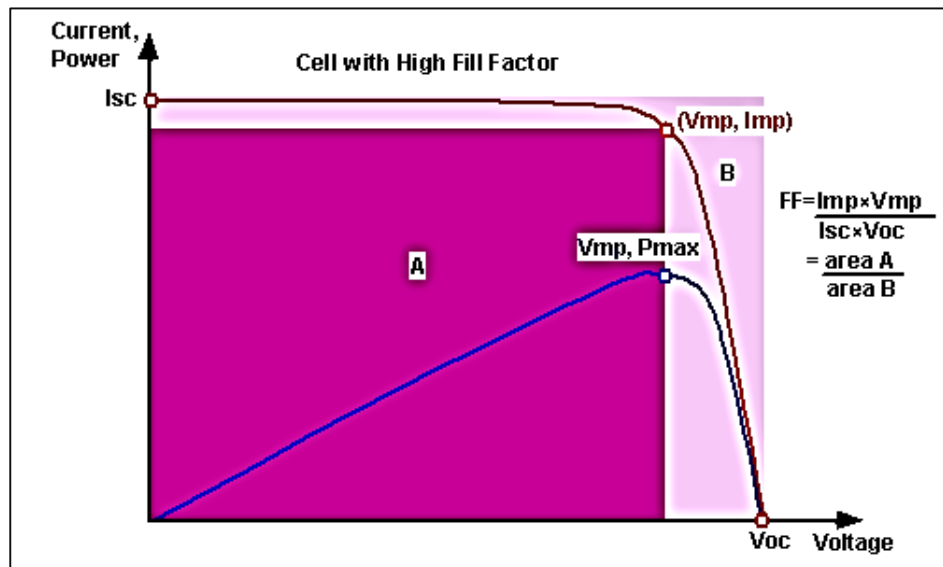


Figure 1.13 Fill Factor (FF) for IV-curve

## 1.9.4 Efficiency

The efficiency defines the working and effective performance of solar cell performance in comparison to another. Efficiency is basically being defined as the ratio of solar cell energy output to solar energy input. The efficiency depends on the spectrum, intensity of the light from the sun, and solar cell temperature of the incident light [13].

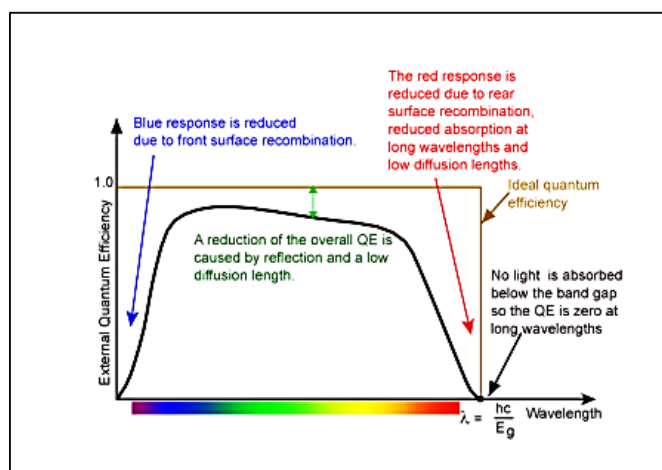


Figure 1.14 Efficiency for IV-curve [13]

## 1.10 Perovskite Solar Cell (PSC)

A class of materials known as halide perovskites has demonstrated potential for solar cells with great performance and cheap production costs. Although other varieties of non-halide perovskites. In comparison to the most popular photovoltaic (PV) technologies, perovskite solar cells have shown comparable power conversion efficiencies (PCE) with the potential for improved performance [15].

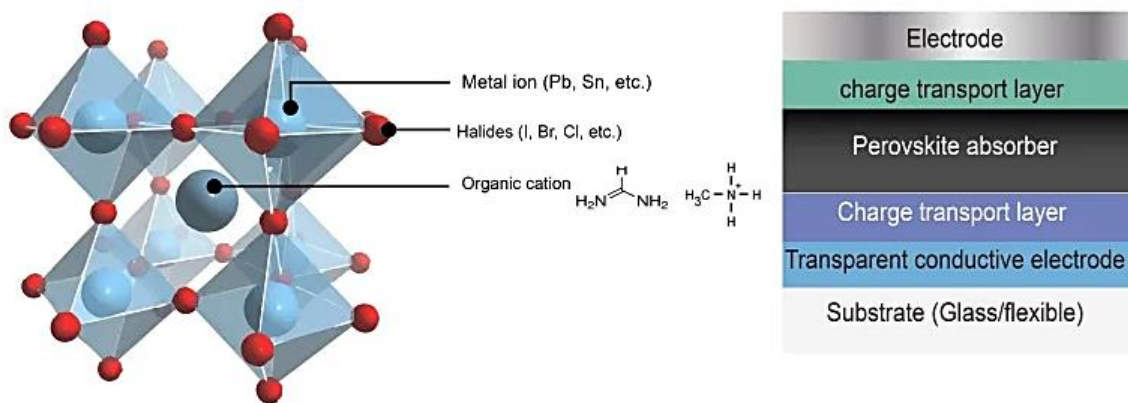


Figure 1.15 Perovskite solar cell crystal molecular structure and multilayers structure [15].

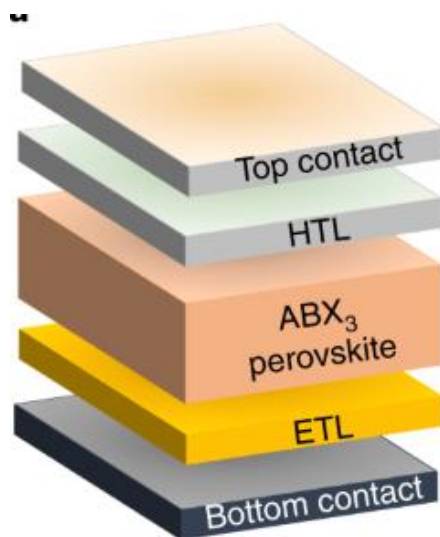


Figure 1.16 Perovskite Solar cell structure [15]

### 1.10.1 ETL (Electron Transport Layer) of Perovskite Solar Cell

A layer with strong electron affinity and electron mobility is called an electron transport layer (ETL). In order for holes and electrons to reach the emissive layer in an equal number, HTL is always significantly thicker than ETL. The ETL is the layer through which electrons go from typical nanoparticles of mesoporous metal oxides like TiO<sub>2</sub> and ZnO to mesoscopic perovskite [16].

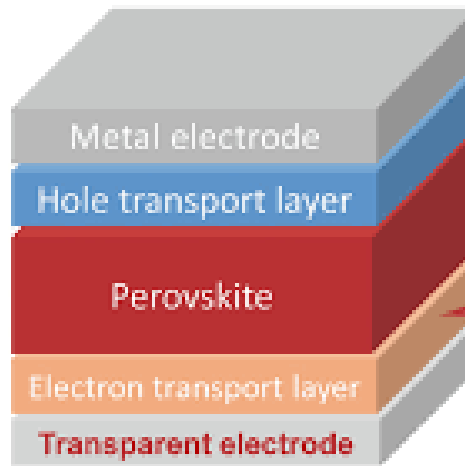


Figure 4.17 Electron Transport Layer in Perovskite Solar Cell [16].

### 1.10.2 HTL (Hole Transport Layer) of Perovskite Solar Cell

In inverted, p-i-n perovskite solar cells (PSCs), hole-transporting layers (HTLs) play a key role in the extraction and transport of holes, surface passivation, perovskite crystallisation, device stability, and cost. Organic HTLs have a number of benefits over that of their inorganic counterparts that being also includes an adjustable band-gap and energy level, simple synthesis and purification, solution processability, and overall cheap cost [17].

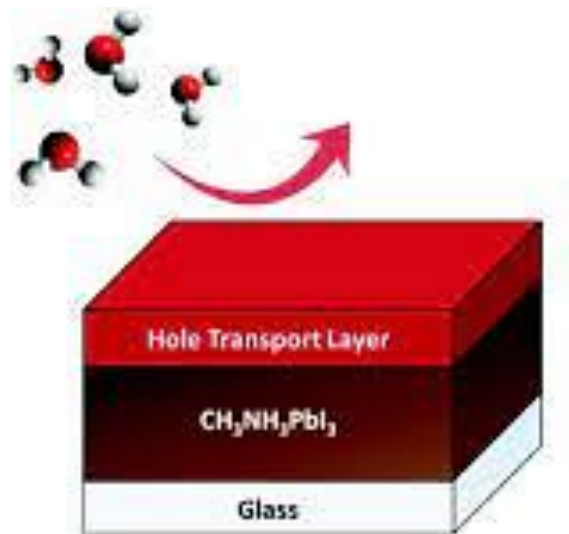


Figure 1.18 Hole Transport Layer in Perovskite Solar Cell [17].

### 1.10.3 Absorber Layer

The semiconducting absorber layer is most frequently being referred to as the brain of all thin film solar cells. The reason behind its vast use is that it is the layer that mostly absorbs the most photons thus, as a result, excites electrons into the conduction band in order to produce photocurrent. Light absorption and carrier extraction are being the main noticing factors. Photocurrent is being produced when a thin layer is being utilised only because there is less absorption, yet the carrier extraction is being the most significant. Even though there are more carriers that were being produced in the device for thick perovskite layers that was mainly due to increased absorption, lower collection efficiency is caused by recombination, that has a major affects Voc [18], [19].

#### **1.10.4 Electrodes**

Electrodes that mainly used for the methy-lammonium lead iodide perovskite solar cell is FTO which is being abbreviated as Flourine-doped Tin based oxide. It is basicallt a type of glass that is usually transparent and conducting. The work function for this type of glass is 0.1eV. It mainly plays role for the extraction of electrons and also for the collection of these electrons.

[20].

#### **1.11 Material of Solar Cell (CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>)**

Solar panels are being made of perovskites that might be easily placed on a variety of surfaces. Due to its simpler production method, cheaper cost, and better flexibility, the main perovskites are frequently being considered to be the most in Solar systems [21].

The TiO<sub>2</sub> electron transport layer (ETL) and Spiro-OMeTAD as Hole Transport Layer (HTL) have a significant impact on the device performance and working in methy-lammonium lead iodide perovskite solar cells abbreviated as (PSCs). Perovskite solar cells made on methylammonium lead/tin tri-iodide (CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/CH<sub>3</sub>NH<sub>3</sub>SnI<sub>3</sub>) are the focus of several ongoing research efforts in the field of photovoltaic. These substances are mainly being found to function as an effective semiconductors. They are particularly applicable when turning photonic energy into electric energy. The band gap of 1.55 almost to 0.01 eV is being applied in the application-relevant room-temperature [21], [22].

The methy-lammonium lead iodide perovskite solar cells structure exhibits excellent photoelectrical features, strong optical absorption coefficients, and a reduced excitation binding energy was being observed. Materials that are with a high dielectric constant make it possible for electrons to be collected

and transmitted efficiently. Perovskite solar cells are excellent solar energy collectors. The materials exhibit high open-circuit voltage VOC and high short-circuit current density. The excitation binding energies of the perovskite materials vary, and as a result, these excitations can either produce free carriers or combine with other excitations. When it is being exposed to sunlight, the perovskite layer basically absorbs photons only by producing electron-hole pairs. [22].

## **RATIONALE**

The scope of the study is to see the effect of variation of temperature of perovskite solar cell and thickness of the provskite layer on the performance of the solar cell by using SCAPS-1D. Methyl ammonium lead halide perovskite solar cells have received a lot of interest recently due to their prolonged charge recombination, strong optical absorption, and longer diffusion length. Due to their high absorption capacity, perovskite materials are perfect for high-performance and reliable solar cell systems. These characteristics make the inorganic-organic perovskite materials ideal for solar cell applications.

## **OBJECTIVE OF THE STUDY**

The main objectives of the study are

- To study and simulate  $\text{CH}_3\text{NH}_3\text{PbI}_3$  based solar cell by using SCAPS-1D.
- To study the effect of varying thickness on the efficiency for the provided structure.
- To study the effect of varying temperature on the efficiency for the provided structure.

## **CHAPTER 2**

### **LITERATURE REVIEW**

Shammas, M, Sofia, T et al. (2023) investigated the performance of the Pb-based perovskite solar cell only by working on the SCAPS-1D. In order to create very effective lead-free n-i-p methyl ammonium tin bromide (MASnBr<sub>3</sub>) perovskite solar cells, this work proposes a modeling-guided device optimisation procedure. We have investigated how different hole and electron transport layers affect MASnBr<sub>3</sub> device performance. Doping concentration of the HTL and ETL, thickness of the perovskite layer, the N<sub>A</sub> and N<sub>D</sub> of the absorption layer and also the defect density. Open circuit voltage, short circuit current, fill factors, theoretical power conversion efficiencies, and quantum efficiencies were being improved using the device glass contact FTO, SnO<sub>2</sub>, perovskite layer MASnBr<sub>3</sub>, front and back contact NiO, Au is suggested here. MASnBr<sub>3</sub> would be used as a perovskite for toxic-free renewable energy [23].

Seyyed, R.H, Mahsa, B et al. (2022) investigated the non-ideal behavior that has major effect on the effective performance of the lead based perovskite using the SCAPS-1D simulation. SCAPS-1D software was being used for the model having FTO as glass contact, TiO<sub>2</sub> as ETL, CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> as provskite layer, Spiro-OMeTAD as HTL. The impact of each of these non-ideal conditions were gradually examined. Also the impact of these parameters named as thickness and doping density were examined in terms of efficiency and recombination in order to optimise each of the essential properties. The results of the stated experimental studies under non-ideal settings during the simulation phase were being checked. This papers check the best thickness and density for the future solar systems. The efficiency was being increased by around 4%. The overall findings showed that the simulated cell is more representative [23].

Kanji, F, Md, Shamsul, A et al. (2022) mainly studied the efficiency that can be enhanced depending on different paramters for lead-based and tin-based that are frequently using perovskite solar cell for varying the HTL and ETL. This was being

carried out using SCAPS-1D. Of all third generation solar cells, the inorganic-organic perovskite solar cell (PSC) holds the most promise for researchers due to its inexpensive manufacturing and quick increase in efficiency. The work was done for the efficiency of the Pb-based and Sn-based perovskite solar cells. This was mainly done by changing ETL and HTL using bandgaps of 1.50 eV and 1.24 eV respectively. The material being used was TCO as ETL, ZnO as HTL, CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>, CuI and Pt as perovskite layer whose efficiency were being observed to be of 23.20% [24].

Mohamed, A, Vishesh, M et al. (2022) studied inorganic or organic based perovskites for their efficiency that would have the major effect on the performance of the solar cell. The work was being done on thin-film thickness and efficiencies for more than 30%. The thickness, donor, defect, and acceptor densities of each thin-films of the solar cells just by using the SCAPS-1D. the work was being observed for power conversion efficiency that basically varies with the operating temperature. The variation of power conversion efficiency with various potential counter electrodes in an effort to substitute the expensive gold counter electrode was being observed. This method was being theoretically use to optimise high-efficiency perovskite solar cells using SCAPS-1D software for solar cells and optoelectronic devices [25].

Qinmiao Chen, YiNi et al. (2022) investigated the perovskite, a novel and promising kind PV solar cell. In this work, a PSC made in ambient air was produced using SCAPS-1D. then, to better comprehend the carrier characteristics, the defect. The perovskite absorber layer's density (Nt), thin film thickness, and energy-level alignment between the electron transport layer (ETL), perovskite absorber layer, and hole transport layer (HTL) were modified. With more Nt, the solar cell operates more effectively. The HTL's valence band is 0.05 eV lower than that of the perovskite absorber layer, which results in a blocking effect that lessens carrier recombination. [26].

Manala, T. M. Davy, M.M et al. (2021) basically studied the thermal instability of the perovskite absorber layer for the halides by using SCAPS-1d. The main focused point was that PSCs also faces thermal instability which leads PSCs towards the

main degradation of the performance of the solar cell. This became the utmost challenge for the researchers to work on the thermal stability of the solar cell and suggest the best remedy for the active performance. The study was being carried out with the analysis of different HTL (hole transport layer) and ETL (electron transport layer). The effect of the doping of the electron transport layers (ETLs) and hole transport layers (HTLs) was being studied and their effect was also observed on the performance of the solar cell which mainly effects the thermal instability. [27].

R. Talaighil Zair, C. Oudjehani and K. Tighilt et al. (2021) studied the tin based perovskite solar cell. The research was being proceeded by using the software SCAPS-1d. This is the most widely used software designed only for the simulation of the solar cell to study and analyze their performance. In this work, we developed a perovskite solar cell based on tin with the innovative architecture Au/CH<sub>3</sub>NH<sub>3</sub>SnI<sub>3</sub>/TiO<sub>2</sub>/ZnO: Al. The SCAPS-1D solar cell capacitance simulator, which is ideally suited to explore the behaviour of solar cells, was used to run a simulation. By inputting a wide range of different parameters into the software tool, we have investigated the impact of the absorber layer thickness and the operating temperature of the model. The acquired ideal parameters are used to forecast the positive findings of: 20.08% conversion efficiency, 32.76mA/cm<sup>2</sup> short-circuit current density (J<sub>sc</sub>), 0.827 V open circuit voltage (V<sub>oc</sub>), and a fill factor (FF) of 74.06%. The outcomes show a strong aptitude [28].

Xiaoming Dou and Yamaguchi, Y et al. (2021) examined is the perovskite solar cell (PSC) by using SCAPS-1D. different parameters were being studied and also their effect on the performance of the perovskite solar cell was being observed under a set temperature. This was being done by changing the doping values and thickness of the electron transport layer (ETL), perovskite absorber layer, and hole transport layer (HTL) were then changed in the perovskite absorber layer in order to better understand the main carrier characteristics that effects the performance of the solar cell. it was observed that the higher value of the defect when used the working performance of the solar cell was effectively increased when it was operated in the presence of the light. The voltage was being set to a certain value such as 0.05 eV

lower than that of the perovskite absorber layer, which results in a blocking effect that lessens carrier recombination. Temperature change and adding defect density were observed that showed that the performance of the solar cell being hindered and degraded by increasing these factors [29].

Nacereddine Lakhdar, Abdelkader Hima et al. (2020) studied the main effect of ETL on the effective performance of the perovskite solar cell which has the absorber layer  $\text{CH}_3\text{NH}_3\text{GeI}_3$  and  $\text{CH}_3\text{NH}_3\text{PbI}_3$ . The study is SCAPS-1D software based. It was being investigated that the various electron transporting layer (ETL) materials has a major effect on the design of mainly used Ge-perovskite solar cells. It had been showed that, in comparison to other ETL materials lead and Germanium-based perovskite solar cells have a power conversion efficiency of 13.5%. Therefore, adding different ETL layers to the design of perovskite solar cells may be regarded as novel designing for later Pb and Ge-perovskite solar cells. Utilising the 1D-Solar Cell Capacitance Simulator (1D- SCAPS), numerical simulation was being carried out [30].

Abdelkader Hima, Nacereddin Lakhdar et al. (2020) studied the parametric effect of diggerent paramters on the performance of the solar cell and observed the immense effect on the performance and working of the solar cell. The efficiency and stability of the absorber perovskite layer  $\text{CH}_3\text{NH}_3\text{GeI}_3$  observed to be degraded by the change of the thickness and other doping of the mainly used materials (perovskite). It was being observed by using HTL different materials such as  $\text{CuSbS}_2$ . Numerical simulation of perovskite solar cells based on methyl-ammonium germanium tri-iodide was being done by running it through the software SCAPS simulation programme. The most efficient strategy to increase device performances is to improve the device's structure and the materials used for both electron and hole transport. The efficiency and stability of  $\text{CH}_3\text{NH}_3\text{GeI}_3$ -based perovskite solar cells was being improved by using a variety of HTMs, including organic and inorganic compound. The most appropriate HTM among the suggested materials is copper antimony sulphide ( $\text{CuSbS}_2$ ). The efficiency was being greatly improved when  $\text{CuSbS}_2$  is used as the HTM in perovskite solar cells,  $\text{CuSbS}_2$  is a

great contender for enhancing the performance of Ge-perovskite solar cells as a consequence of the results that were achieved [31].

S. Karthick, S. Velumani et al. (2020) studied the comparison mainly for different lead based materials that effect the performance of the perovskite solar cell. Comparison was being done for the photovoltaic performance of methylammonium-free perovskite solar systems based working of the solar cell by using the software SCAPS-1D for simulations. The doping valued were being varied for cesium and bromide and observed that there is an increase in the power conversion efficiency (PCE) of related devices from 4 to 15% when it was being exposed to ambient light. By utilising the SCAPS-1D programme to analyse the electrical properties of the cell as a function of active layer composition, the impact of series and shunt resistances (&) was theoretically assessed and discussed. The experimental trends are not matched by ideal devices, despite the fact that they did show how the bandgap edge affects photocurrent production. It was being interpreted that the key constraints on the device current-voltage characteristics by feeding the experimental data and values to SCAPS. A decrease in the parametric value of fill factor (FF) was being observed. The results unequivocally support the positive impact of mixed cations and mixed halides on device performance [32]

## **CHAPTER 3**

### **METHODS AND MATERIALS**

#### **3.1 SCAPS**

SCAPS (Solar Cell Capacitance Stimulator) is a widely used one-dimensional simulation program. This software is used for Solar cells for measuring efficiency by varying different factors and getting results by plotting the graph. It was developed by number of developers. Initially used for perovskite solar cells such as  $\text{CuInSe}_2$  and  $\text{CdTe}$ .

#### **3.2 Characteristics of SCAPS**

**Following are the main characteristics of the SCAPS**

- It can be used to add several layers structure i.e maximum seven layers of semiconductor.
- The working point can be specified for voltage, frequency, and temperature calculations.
- At the working point, the software calculates currents, concentrations, and bands.
- Software can be run using a scripting language feature.

#### **3.3 Getting started with SCAPS**

##### **3.3.1 Basics of SCAPS**

Since SCAPS was developed using Lab Windows, it is geared toward Windows. "Panel" is the name of a page that opens in SCAPS. The basic work is divided into clearly defined panels.

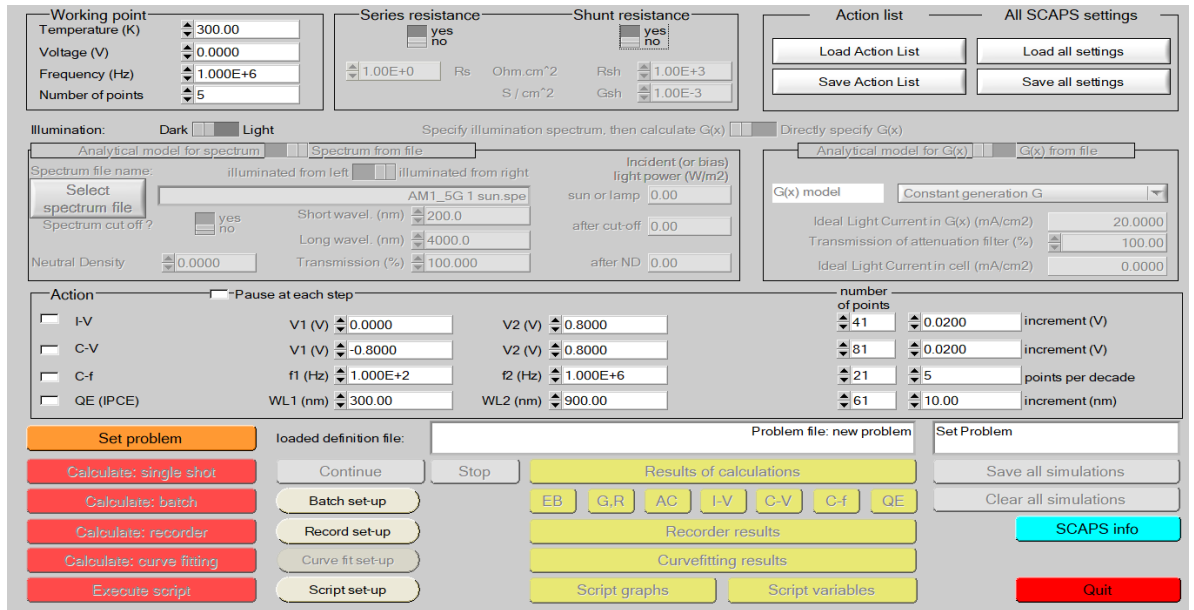


Figure 3.1 Action Panel of SCAPS

### 3.3.2 Run SCAPS

- Include details about the solar cell's material, geometry, and problem definition.
- Specify the circumstance under which simulation will be carried out.
- Start the calculations.
- Display the simulated graphs.
- Run SCAPS after defining the measurement that will be simulated.

Double-click SCAPS 3200.exe or any other version in the file folder. Software will launch using the Action Panel.

### 3.3.3 Define the Problem

A button labeled "set problem" can be found in the panel. Click this button to characterize your issue. All attributes of cell can likewise be changed later.

### 3.3.4 Define the Working Point

- It characterizes the variables which are connected with estimations yet are not inconsistent.

- Temperature T is connected with all estimations. The temperature, thermal voltage, and velocities in this program are not only variables but also depend on all of their derivatives.
- Voltage is disposed of into C-V and I-V reproductions. In simulations of quantum efficiency, it would be direct voltage. Zero is always the voltage at the beginning. Recurrence is excluded from all reproductions with the exception of C-V.
- Enlightenment is utilized in all estimations.

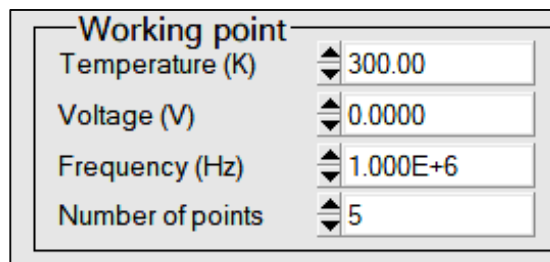


Figure 3.2 Action Panel of SCAPS

### 3.3.5 Select the measurements to stimulate

One or more measurements can be chosen to be used in the simulation of all variables. One simulation can be performed at a time.

### 3.3.6 Start the Calculations

Click the button to calculate the single shot, and the panel of energy bands will open. A line at the panel's bottom depicts the simulation process.

### 3.3.7 Display the stimulated curves

SCAPS will open the interface for energy band board after the computations. Diagrams of energy bands, charge carrier densities, and current are displayed on this panel. By clicking the save graphs button, the user can save the results.

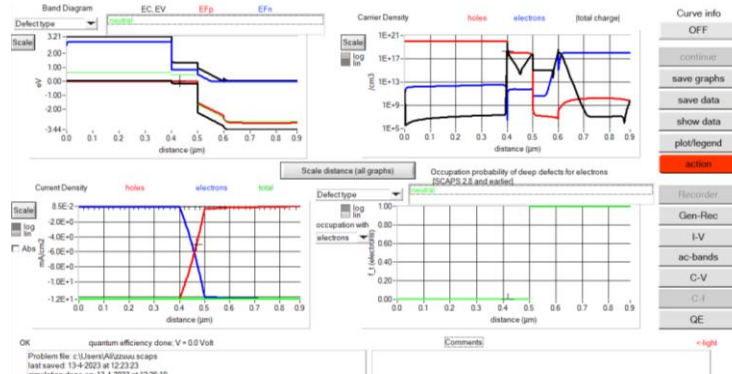


Figure 3.3 Stimulated curves in SCAPS

### 3.3.8 Editing the Problem

The problem can be edited or changed by the user only by clicking on the set problem that appears in the interface of the Action Panel.

## 3.4 Solar cell definition

### 3.4.1 Editing a solar cell definition

The panels to define the solar cell open when you click the set problem from the action panel. This permits client to alter the designs.



Figure 3.4 Solar cell definition

### 3.4.2 References convention for the voltage and current

The user can easily change the current and voltage. A problem would not contain any references when it was set or edited.



Figure 3.5 Numerical setting Panels

Three additional facilities have been added;

- Apply voltage  $V$  to; when the user sets the left contact, voltage will be applied to the left contact; when the user sets the right contact, voltage will only be applied to the right contact.
- Current reference, in that when the user selects the consumer, the current reference's arrow is set to something like  $P=JXV$ . Cell uses this as its source of power.
- The x-axis is the direction along which the solar cell construction can be reversed. You may get the original structure by pressing the inversion button twice.

### 3.4.3 Contacts

The contact properties might be determined from the definition of the solar cell panel. The user can use from flat bands or the metal work feature. When an intrinsic layer is present, when an n-type layer is employed, or when a p-type layer is used.

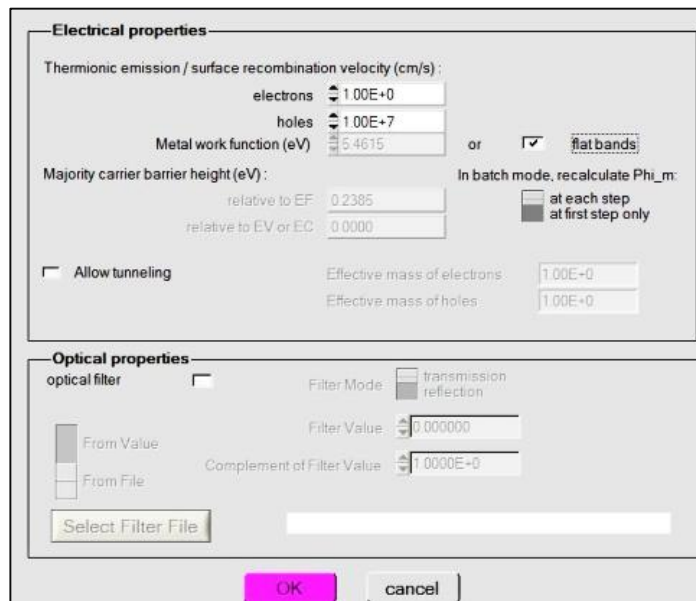


Figure 3.6 Left contact in Solar cell definition panel

### 3.4.4 Layer thickness

The definition of layer thickness in SCAPS prior to version 3.3, 2014, used micrometres. The latest SCAPS versions that came out after 2014 enable the usage of nanoscale units (nano-meters).

### 3.4.5 The constant layer of an optical absorption

SCAPS uses simple files, sometimes referred to as ASCII files. These files are designated with the .abs extension. It offers a collection of .abs files useful for modelling.

### 3.4.6 A material approach

The user of this programme may individually describe each variable for each layer. By selecting the "load and save material" option, this programme is permitted to load and store the settings to a file of material.

#### 3.4.6.1 Saving materials

Four alternatives can be utilised to store any substance, including pure A and pure B, both materials, and pure Y. Only the factors of the layer's pure A/B material will be saved if a user chooses to save just that.

### **3.4.6.2 Loading material**

There are three alternatives for the material load: pure A, pure B, or both. When the user selects one of the two materials as their sole options, the A/B parameters are loaded.

### **3.5 Illumination conditions**

The more criteria that may be provided, the better when simulations are run under lighting circumstances. The user may select the spectrum, side of lighting, and light or dark.

### **3.6 Internal SCAPS calculation**

SCAPS also enables you to run simulations for your own structure's generation calculations. It is possible to change the illumination's side. There are two types of monochromatic spectrum, such as those with illumination of 20mA/cm or 1000w/m total power. The spectrum file initially has a line of wavelengths numbers. Two columns make up the first line; one column contains the wavelength (nm), while the other column contains the power of incidence [33]

- There are no reflections that can be implemented at interfaces.
- The power of incidence could only be changed by applying a density filter.

### **3.7 The generation models**

#### **3.7.1 Constant generation G**

There is just one parameter of G that is utilised to express photon flow and current. For calculating cell thickness, this model of generations is employed. This generation will alter based on thickness.

#### **3.8 Shunt conductance and series resistance**

The user is allowed to use series and shunt resistance from the Action Panel. Both can be easily used at a time and thus conductance can easily be defined.

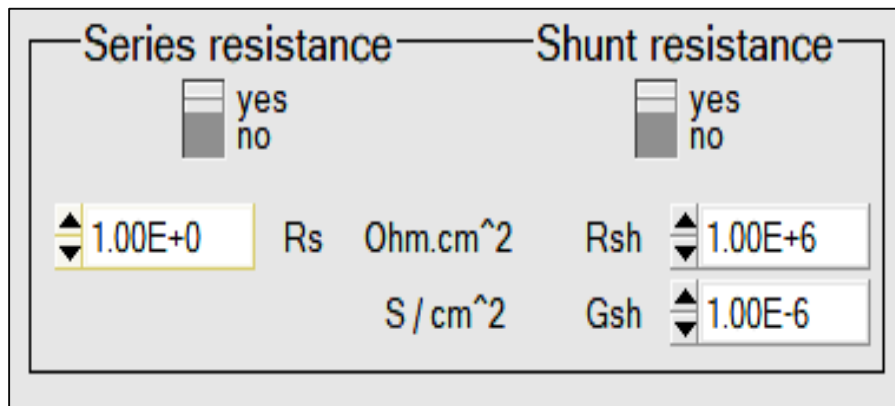


Figure 3.7 Panel of shunt conductance and series resistance

### 3.9 Navigating the analysis

The user can use the action panel's navigation panel. There are a few choices available in each panel, including save, show data, and graphs. Some are particular panels.

### 3.10 Curve info and legend

The graph would be overcrowded if simulations were to be run. By selecting the plot/legend button, the curves on graphs can also be hidden or shown.

### 3.11 I-V panel

The results of current and voltage simulations are displayed in this panel. All current and voltage simulations are shown on the left graph, while information on the most recent simulation's currents is shown on the right graph. Short circuit current would be exactly produced when voltage was adjusted to 0. The I-V graph is also shown as I (V) graph, but short circuit current may be increased or decreased by altering the current modes.

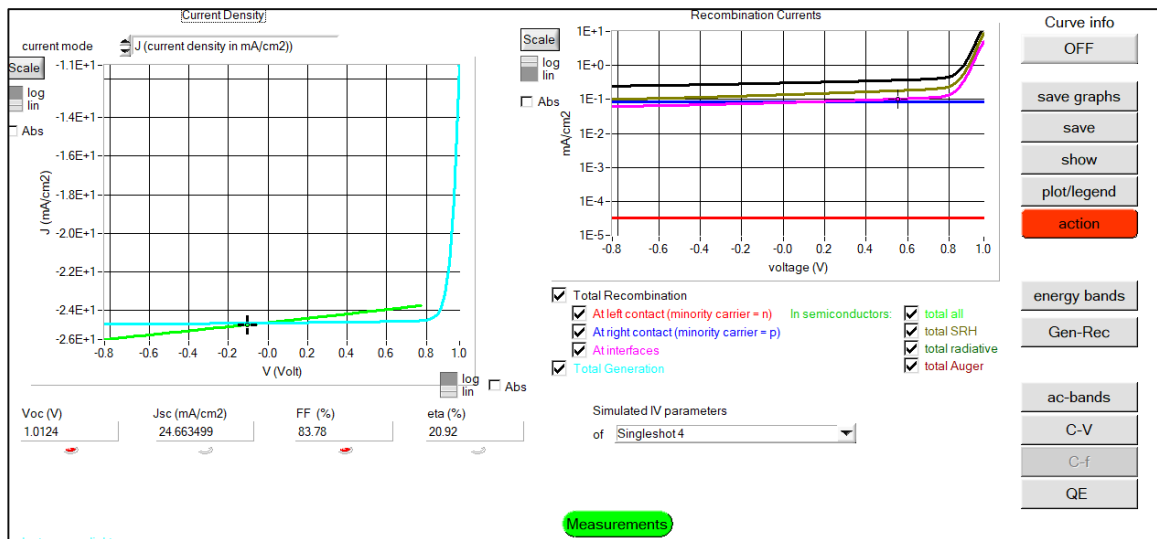


Figure 3.8 I-V Panel [33]

### 3.12 Introduction to Origin

Origin is the most powerful data analysis and graphing programme designed specifically for scientists and engineers. The simplicity with which you can personalise and automate your data import, analysis, graphing, and reporting chores is what distinguishes Origin from other apps. [34]

### 3.13 Characteristics of Origin

Following are the main characteristics of Origin

- It can be used for different forms graph plotting.
- Several types of fitting can easily be performed using origin such as Curve fitting, Surface fitting and peak fitting
- Multi-panel graph can easily be plotted for the basic comparison and analysis.
- Signal processing and image processing are the key features of the Origin.

### 3.14 Getting started with Origin

#### 3.14.1 The Basics

Since Origin was developed using Lab Windows, it is geared toward Windows interface. "workbook", "worksheets" are the name of a page that opens in Origin [33]

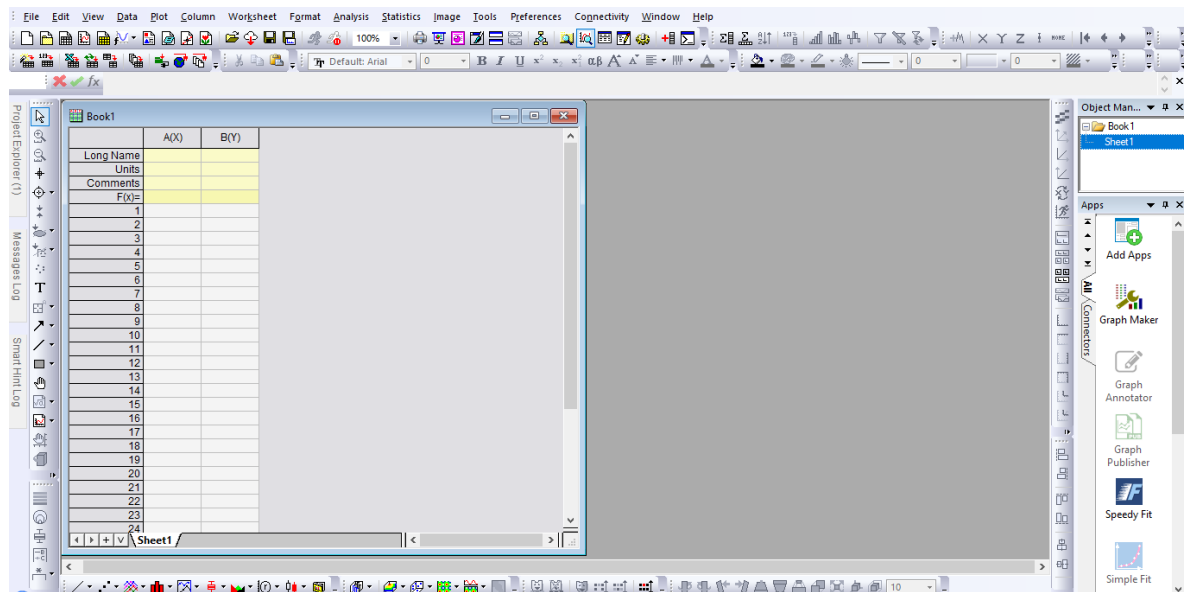


Figure 3.9 Workbook interface in Origin [34]

### 3.14.2 Run Origin

- In the first step, open Origin a workbook appears then select the values or import the values for the x or y columns.
- In the second step, name the columns with a variable or the name for the selected parameter.
- In third step, write the unit for the selected parameters.
- For the plotting purposes, select the columns between which the graph is to be plotted.
- Then click the plot.
- Select the type of plot that depends on the requirement of the results.
- The graph is being plotted.

### 3.14.3 Define the Parameters

As the workbook interface appears, shows the columns as A(X) and B(Y). You can add more columns by clicking on columns and insert. Name the columns with selected parameters. [34]

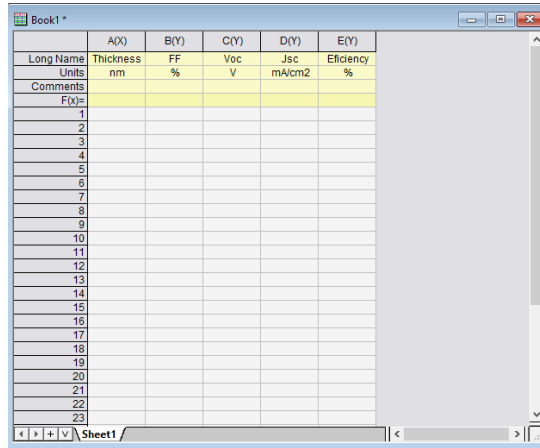


Figure 10 Defining the Parameters [34]

### 3.14.4 Setting the values and Columns

Copy or import the values from the required file into the Columns.

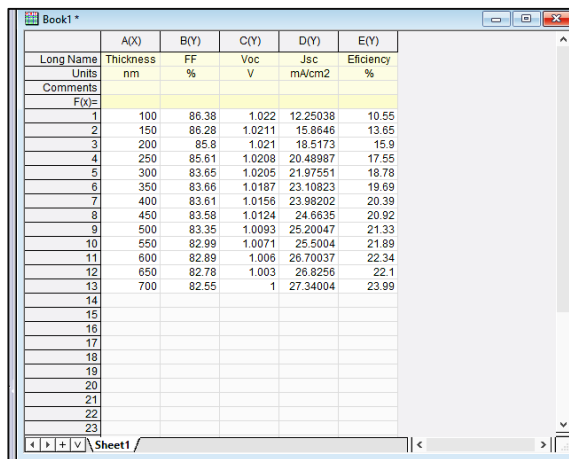


Figure 11 Setting values in Columns [33]

### 3.14.5 Start Plotting

Plotting can be done by selecting the parameters between with analysis is to be done first, then right click and select plot. Now select the type of plot.

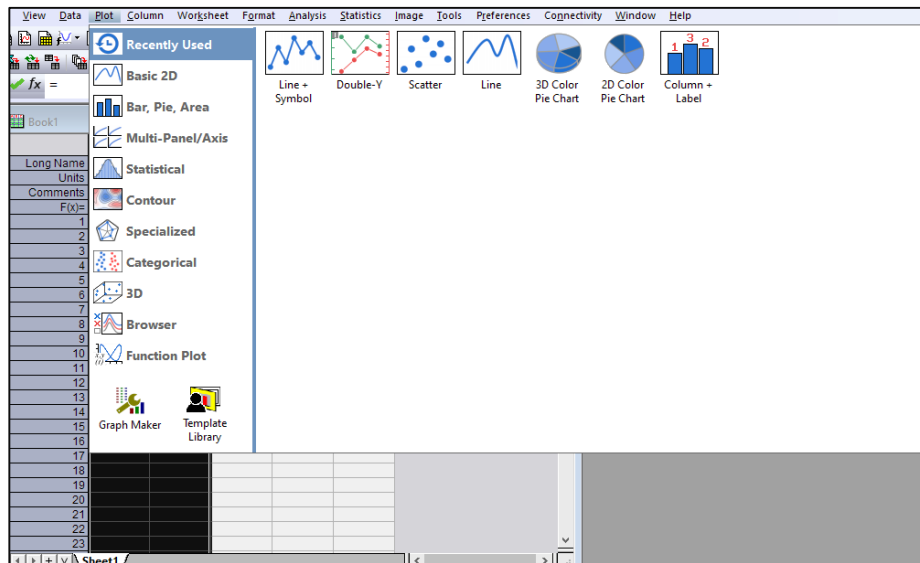


Figure 12 Plotting panel

### 3.15 Graph interface

The graph interface appears after the parameters being plotted. The graph interface shows the x-axis and y-axis.

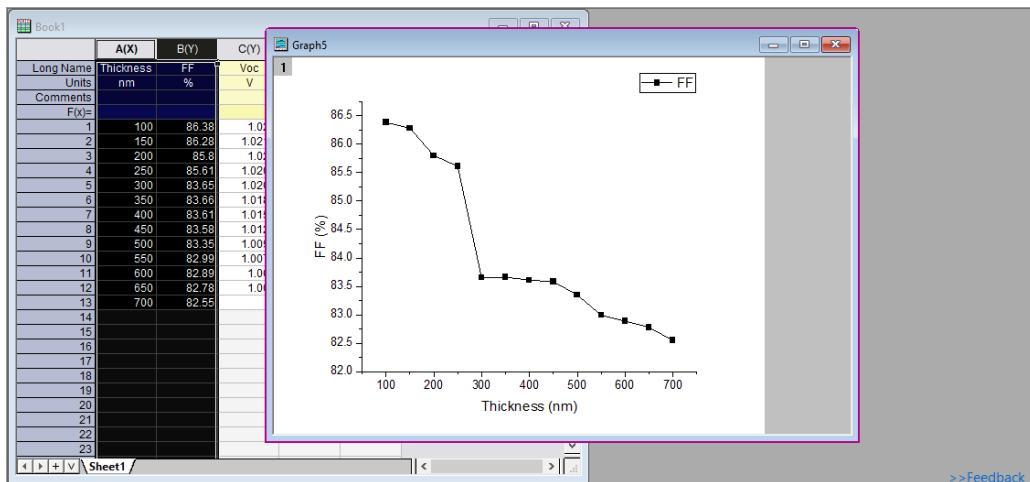


Figure 13 Graph Interface [34].

#### 3.15.1 Editing the axis

The axis such as x and y can be edited by double clicking on the x-axis and y-axis, an action pane appears. This lead us to change the values and scale of axis.

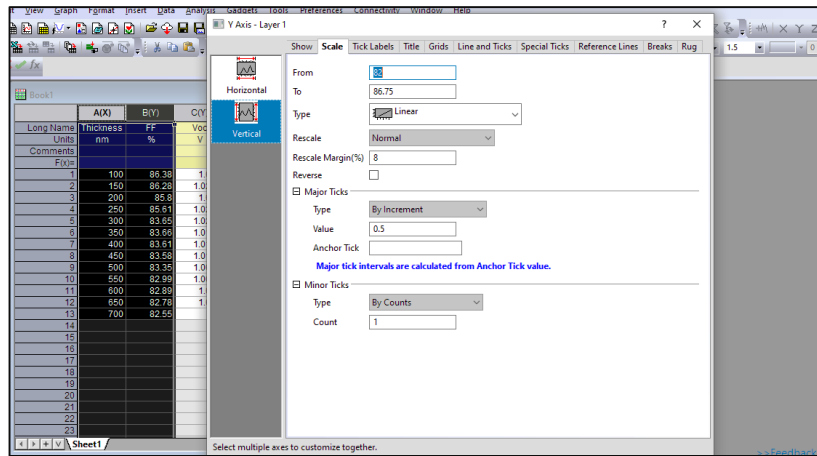


Figure 14 Axis action pane

### 3.15.2 Saving the graph

The graph can be save by right clicking on the graph interface, the select the export graph and select the type in which you want to save the graph. [34]

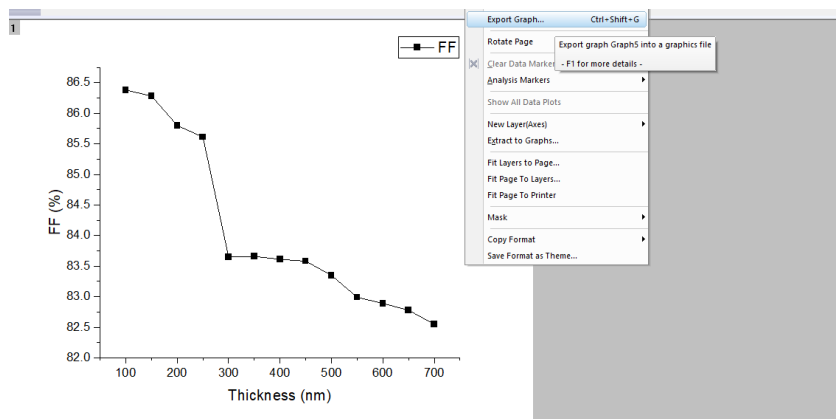


Figure 15 Exporting graph

Click ok. Thus your graph will be exported.

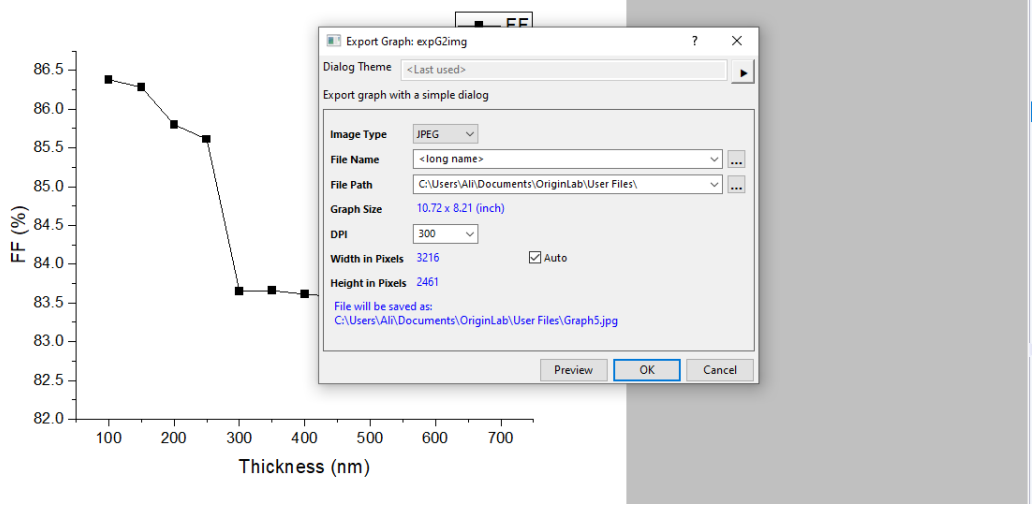


Figure 16 Selecting type for exporting graph [33]

## CHAPTER 4

### RESULTS AND DISCUSSION

The Department of Electronics and Information Systems (ELIS) at the University of Gent in Belgium created SCAPS-1D, or "Solar Cell Capacitance Simulator one Dimension," a one-dimensional solar cell simulation programme. A software programme called SCAPS has several panels on which the user may enter various solar cell properties. The outcomes are computed and illustrated. The action panel, solar cell definition panel, and energy band panel are the three main panels. The study is carried out in which two parameters the thickness and temperature are varied and thus their effect the performance of the solar cell is being observed. The ETL (electron transport layer) is  $\text{TiO}_2$  with thickness 50nm and HTL (hole transport layer) is Spiro-OMeTAD with a thickness of 500nm is used.  $\text{TiO}_2$  is being used because its structure is so simple, it has high thermal stability, its nature of being highly compatible with flexible substrates. Spiro-OMeTAD is used because of its high efficiency, stability and high performance in electrical devices.

#### 4.1 $\text{CH}_3\text{NH}_3\text{PBI}_3$



Figure 4.1 Schematic structure of  $\text{CH}_3\text{NH}_3\text{PBI}_3$

The Methylammonium Lead Iodide ( $\text{CH}_3\text{NH}_3\text{PBI}_3$ ) Perovskite Solar Cell has Produced a Remarkable Breakthrough in the Photovoltaic History of Solar Cell Technology. It is basically a metal halide perovskite with a large band gap that is appropriate for solar cells with high open-circuit voltage ( $V_{oc}$ ) and belongs to the

class of organic-inorganic halide perovskites (OIHPs) with outstanding electrical and optical (photovoltaic) properties appropriate for solar applications.

Table 4.1 Parameters of CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> [30],[33]

<b>Parameters</b>	<b>CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub></b>
Thickness (um)	100-700nm
Band Gap (eV)	1.550
Electron Affinity (eV)	3.900
Dielectric permittivity (relative)	30.000
Electrons in CB (cm <sup>-3</sup> )	2.500E+20
VB (cm <sup>-3</sup> )	2.500E+20
Electron Thermal Velocity (cm/s)	1.000E+7
Hole Thermal Velocity (cm/s)	1.000E+7
Electron mobility (cm <sup>2</sup> /Vs)	5.000E+1
ND (cm <sup>-3</sup> )	0.000E+0
NA (cm <sup>-3</sup> )	1.000E+18

Table 4.2 Parameters of TiO<sub>2</sub>, Spiro-OMeTAD and FTO [33]

<b>Parameters</b>	<b>Spiro-OmeTAD</b>	<b>TiO<sub>2</sub></b>	<b>FTO</b>
Thickness (nm)	450	50	280
Band Gap (eV)	3.170	3.260	3.500
Electron Affinity (eV)	2.100	4.200	4.000
Dielectric permittivity (relative)	3.000	10.000	9.000
Electrons in CB (cm <sup>-3</sup> )	2.000E+18	2.000E+18	1.000E+19
VB (cm <sup>-3</sup> )	1.800E+19	1.800E+19	1.000E+18

Electron Thermal Velocity (cm/s)	1.000E+7	1.000E+7	1.000E+7
Hole Thermal Velocity (cm/s)	1.000E+7	1.000E+7	1.000E+7
Electron mobility (cm <sup>2</sup> /Vs)	2.000E-4	2.000E+1	2.000E+1
Hole mobility (cm <sup>2</sup> /Vs)	2.000E-4	1.000E+3	1.000E+1
ND (cm <sup>-3</sup> )	0.000E+0	1.000E+15	1.000E+18
NA (cm <sup>-3</sup> )	1.000E+20	0.000E+0	0.000E+0

## 4.2 Effect of thickness

The simulation is being performed under the optical environment and the calculation of the solar cell parameters are done. The thickness of the layer CH<sub>3</sub>NH<sub>3</sub>PBI<sub>3</sub> was varied between 100 to 700nm with a difference of 50.

### 4.2.1 Effect of thickness on open circuit voltage (Voc)

As the perovskite thickness increases the open circuit voltage decreases. The reason for the decrease of the Voc is that the saturation current is basically in the opposite to that of the illumination current and also because of the expansion of the absorption layer. When the thickness of the layer is thin Voc is large.

Table 4.3 Values for Voc with increase of thickness

THICKNESS (nm)	Voc (V)
100	1.0120
150	1.0211
200	1.0010
250	1.0008
300	1.0215
350	1.0187
400	1.0156
450	1.0124

500	1.0093
550	1.0071
600	1.006
650	1.003
700	1

The table 4.3 shows the decrease of Voc with the increase of perovskite layer thickness which is graphically displayed in figure 4.2.

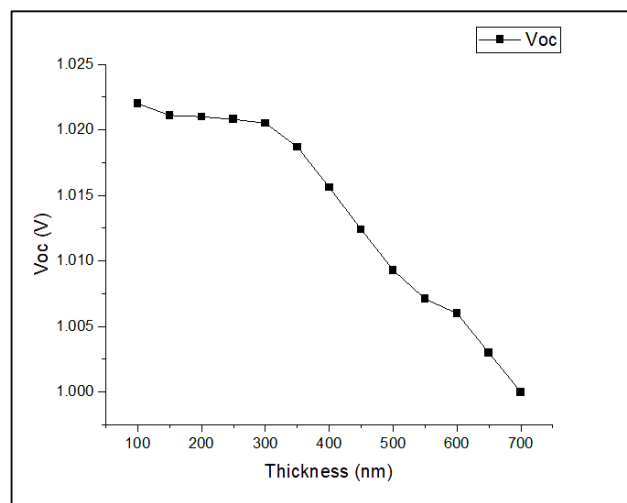


Figure 4.2 Effect of increase of the thickness of perovskite layer on the open circuit volage (Voc)

#### 4.2.2 Effect of thickness on current density (Jsc)

As the perovskite thickness increases the current density increases. For the current density graph we can say that by increasing the thickness of the perovskite layer the short circuit current increases because of the increase of the spectral response to the longer wavelength.

Table 4.4 Values of Jsc with the increase of thickness

THICKNESS (nm)	Jsc (mA/cm <sup>2</sup> )
100	12.250380

150	15.8646
200	18.517296
250	20.489871
300	21.975514
350	23.108234
400	23.982021
450	24.663499
500	25.200468
550	25.200402
600	26.82522
650	26.8356
700	27.34004

The table 4.4 shows that the  $J_{sc}$  increases with the increase of the thickness of the perovskite layer which is being graphically represented in figure 4.3.

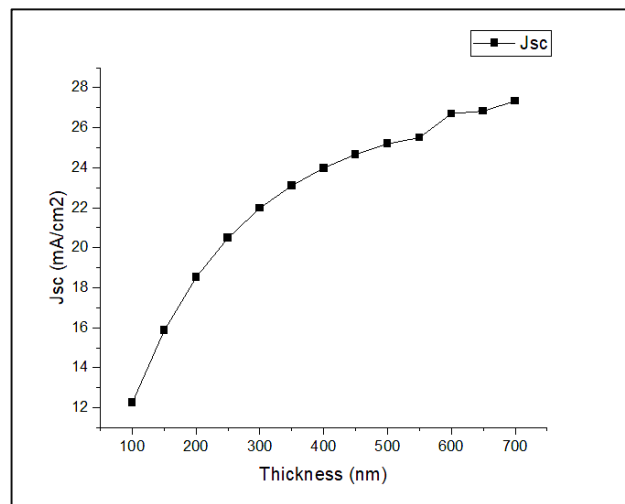


Figure 4.4 Effect of increase of thickness of the perovskite layer on the current density or short circuit current Jsc

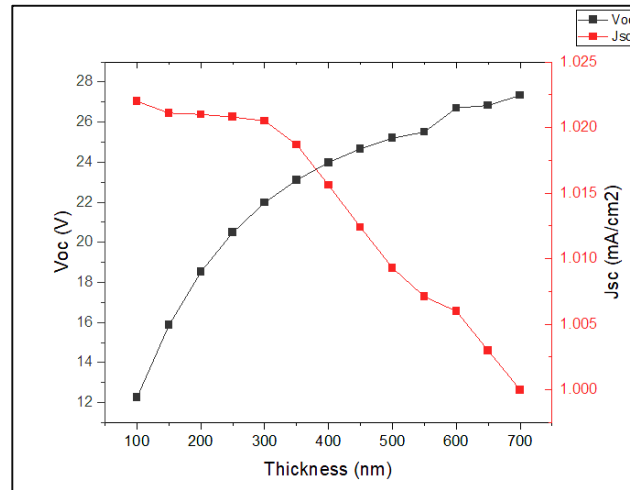


Figure 4.5 comparison of the increase of the perovskite layer thickness on the open circuit voltage (Voc) and current density or short circuit current (Jsc).

The increase in the thickness of the layer of perovskite cause an increase in the short circuit current (Jsc) and decrease in the open circuit voltage (Voc).

### 4.2.3 Effect of thickness on FF (fill factor)

As the perovskite layer thickness increases the FF% decreases.

Table 4.5 Values of FF (fill factor) with increase of thickness

THICKNESS (nm)	FF%
100	86.38
150	86.28
200	85.95
250	85.61
300	85.3
350	84.99
400	84.6031

450	84.2
500	83.6
550	83.1
600	82.89
650	82.6
700	82.4

The table 4.5 shows that the increase of the perovskite layer thickness causes decrease of the fill factor which is being graphically represented in the figure 4.6.

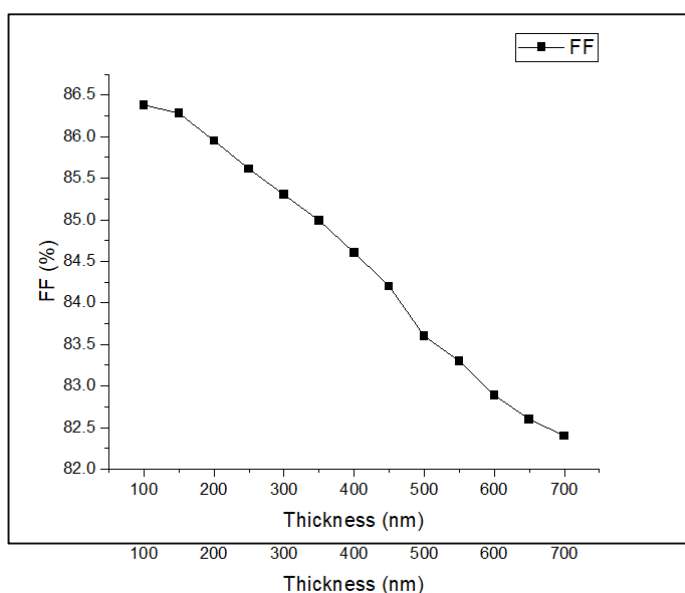


Figure 4.6 Effect of the increase of thickness of the perovskite layer on the FF (fill factor).

#### 4.2.4 Effect of thickness on the Efficiency %

As the perovskite layer thickness is varied the performance of the solar cell is affected. The increase of the perovskite layer's thickness cause increase in the efficiency of the solar cell. This is because the movements of inner atoms increases

at higher temperatures. Causing atoms to vibrate more readily, thus the efficiency increases.

Table 4.6 Effect of thickness increase on the Efficiency

THICKNESS (nm)	EFFICIENCY (eta) %
100	10.55
150	13.65
200	15.90
250	17.55
300	18.78
350	19.69
400	20.39
450	20.92
500	21.33
550	21.33
600	21.89
650	22.1
700	23.99

The table 4.6 shows that the increase of the thickness of the perovskite layer cause increase of the efficiency of the solar cell which is graphically being showed in the figure 4.7.

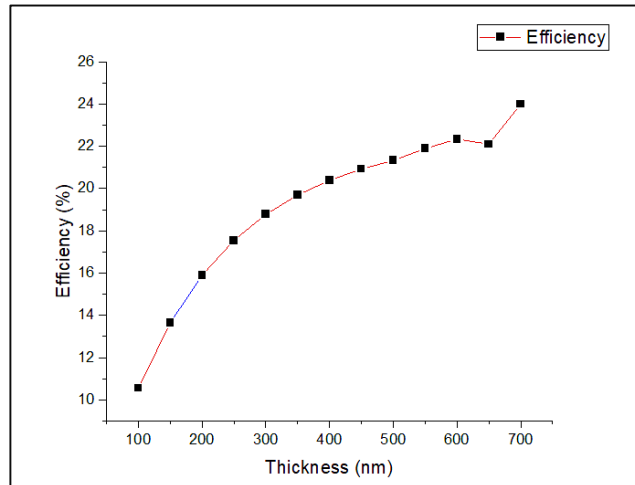


Figure 4.7 Effect of the increase of the thickness of the perovskite layer on the efficiency

### 4.3 Effect of temperature

Solar cells are being very sensitive to the temperature. The best working temperature for the solar cell is 300K. As we know that solar cells are being used in Sunlight under such conditions the temperature will definitely increase and the performance of the solar cell will be degraded.

#### 4.3.1 Effect of temperature on open circuit voltage (Voc)

As the thickness of the perovskite layer increases the open circuit voltage drastically decreases.

Table 4.7: Effect of temperature on open circuit voltage (Voc)

Temperature (K)	Voc (V)
300	1.000
350	0.9831

400	0.8034
450	0.7601
500	0.6201

The table 4.7 shows that the increase of the temperature cause decrease in the open circuit voltage because of the increase of the saturation current due to the opposite direction of saturation current to that of the illumination current which is being graphically represented in figure 4.8.

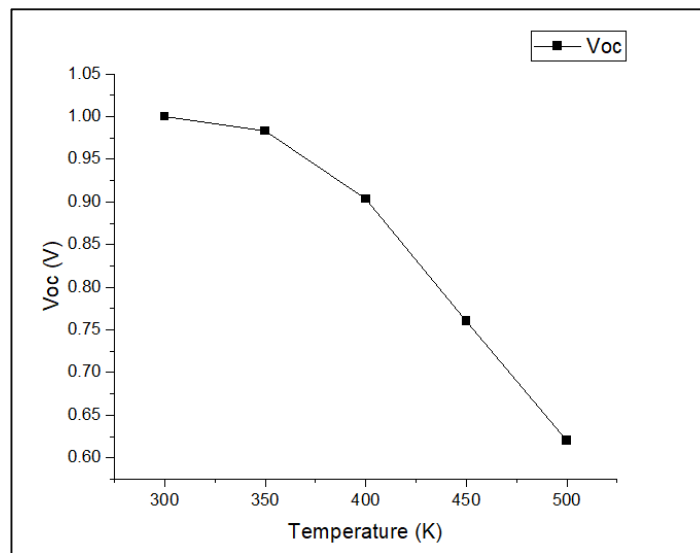


Figure 4.8 Effect of increase of temperature on the open circuit voltage (Voc)

### 4.3.2 Effect of temperature on short circuit current density (Jsc)

As the perovskite layer thickness increases the short circuit current decreases.

Table 4.8: Effect of temperature on short circuit voltage (Jsc)

Temperature K	Jsc (mA/cm <sup>2</sup> )
300	27.34004

350	26.99801
400	26.65306
450	25.86011
500	25.22031

The table 4.8 shows that there is a gradual decrease of the short circuit current as the temperature increases above 300K because at high temperature the vibrational motion of electrons is very high that mainly hinders their motion for maximum current which is being graphically represented in the figure 4.9.

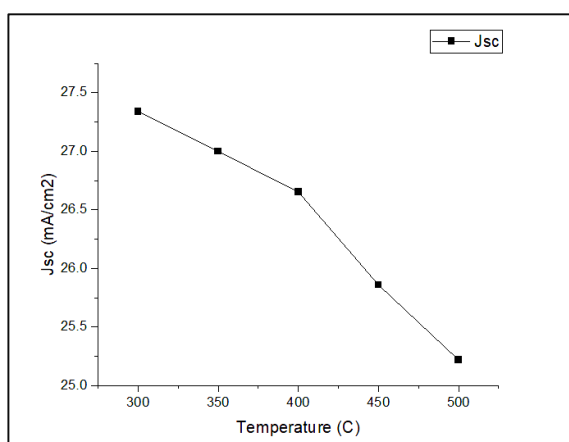


Figure 4.9 Effect of temperature on the short circuit current or current density ( $J_{sc}$ )

### 4.3.3 Effect of temperature on FF % (fill factor)

As the temperature is being increased the fill factor FF% is being decreased

Table 4.9 Effect of temperature on the FF%

Temperature K	FF %
300	82.55
350	80.32
400	79.01
450	72.50
500	69.99

The table 4.9 shows that the fill factor decreases with the increase of the temperature because of the change of  $V_{oc}$  and  $J_{sc}$  which is being graphically represented in the figure 4.10.

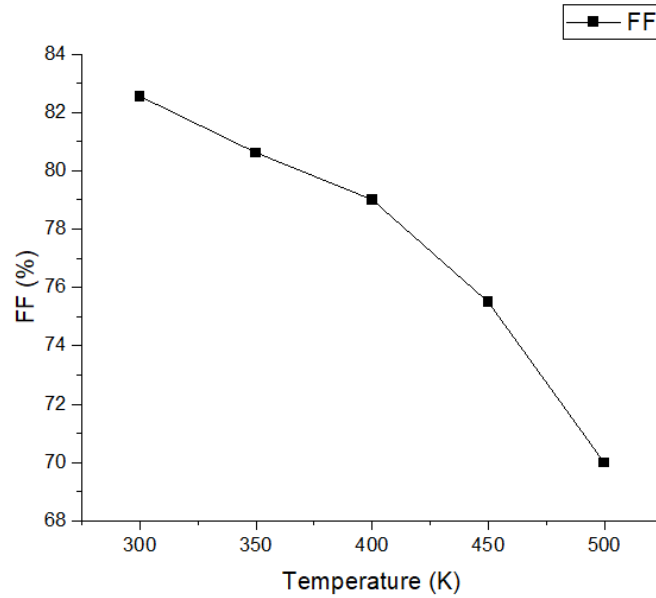


Figure 4.10 Effect of increase of temperature on the (fill factor) FF%.

#### 4.3.4 Effect of temperature on the Efficiency

As the temperature exceeds above 300K the efficiency of the solar cell decreases drastically which shows a great degradation in the performance of the Solar cell.

Table 4.10 Effect on Efficiency with the increase of the temperature

Temperature K	Efficiency (eta) %
300	23.99
350	22.81
400	21.76
450	19.10
500	16.43

The table 4.10 shows that as the temperature increases the efficiency of the solar cell decreases to work effectively. This happens because at higher temperatures, recombination rate of the charge carriers is being increased. This is being graphically represented in the figure 4.11.

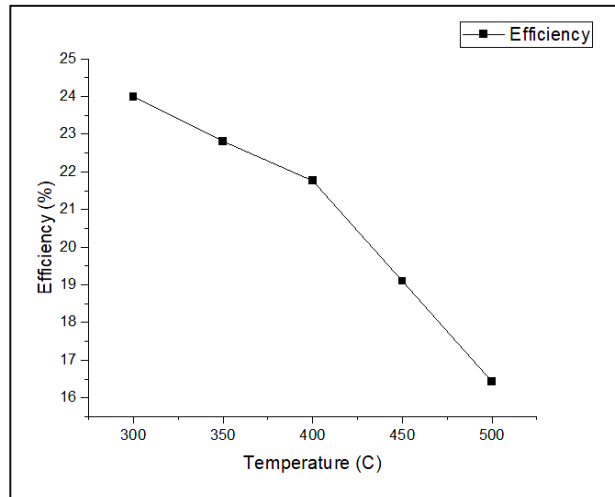


Figure 4.11 Effect of increase of temperature on the Quantum Efficiency

## CONCLUSION

Lead based perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$  has been simulated using SCAPS-1D. The main parameters that are observed are thickness and temperature. When these parameters are varied changes are observed in the performance of the solar cell. The increase in the thickness cause decrease of short circuit voltage  $V_{oc}$  from 1.0220 V to 1.0000V, increase in Short circuit current  $J_{sc}$  from 12.25mA/cm<sup>2</sup> to 27.34mA/cm<sup>2</sup>, decrease in FF% from 86.38% to 82.55% and increase in efficiency from 10.55% to 23.99%. The increase in the temperature cause decrease in open circuit voltage  $V_{oc}$  from 1.000 V to 0.6201 V, decrease in short circuit current  $J_{sc}$  from 27.34 mA/cm<sup>2</sup> to 25.22 mA/cm<sup>2</sup>, decrease in FF% in 82.55% to 69.99% and decrease in efficiency from 23.99% to 16.43%. For the better performance and efficiency of solar cell the thickness of the perovskite layer must be increase and temperature should be near 300K (as much cool as possible).

## **LIMITATIONS**

- As the available data is limited, the doping effects are not being taken into account.
- Use of lead oxide can create environmental issues.
- High temperatures are the main concern for the degraded performance.
- Availability of parameteric values is not easy to find due to limited literature review.

## **RECOMMENDATIONS**

- Different HTL, ETL material can be used to authenticate the perovskite solar cell for its better performance and efficiency.
- Perovskite solar cell must be used instead of conventional solar cell of conventional one because of the high performance, efficiency and potential for better performance of perovskite solar cell.
- As the high temperature is affecting the performance of perovskite solar cell, for this cooling methods with phase change materials such as nanoparticles or porous metal should be used.
- ETL, HTL and electrodes can be engineered for improving their structure.

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