# SIMULATION AND MODELLING OF SEMICONDUCTOR OPTOELECTRONIC DEVICE (SOLAR CELL)

***A PROJECT REPORT***

***Submitted***

*In the fulfilment of the requirements for*

*the award of the degree of*

**Bachelor of Technology**

**in**

**Electronics and Communication Engineering**

By

| **Dondeti Harsha Vardhini** | **Vedagiri Divya** | **Palugulla Kavya** |
|---|---|---|
| **[201FA05010]** | **[201FA05095]** | **[211LA05042]** |

Under the Esteemed Guidance of

**Dr. Ashutosh Kumar Dikshit**

Assistant Professor

Department of ECE

VIGNAN'S
Foundation for Science, Technology & Research
(Deemed to be University)
-Estd. u/s 3 of UGC Act 1956

**(ACCREDITED BY NAAC WITH 'A+' GRADE)**

**DEPARTMENT OF ELECTRONICS AND COMMUNICATION ENGINEERING**

(ACCREDITED BY **NBA)**

**VIGNAN'S FOUNDATION FOR SCIENCE TECHNOLOGY AND RESEARCH**

**(Deemed to be University)**

**VADLAMUDI, GUNTUR – 522213, INDIA**

**May- 2024**

# CERTIFICATE

This is to certify that the project report entitled **"SIMULATION AND MODELLING OF SEMICONDUCTOR OPTOELECTRONIC DEVICE(SOLAR CELL)"** that is being submitted by **Dondeti Harsha Vardhini [201FA05010], Vedagiri Divya[201FA05095], Palugulla Kavya[211LA05042]** infulfilment for the award of B.Tech degree in Electronics and Communication Engineering, Vignan's Foundation for Science, Technology and Research University , is a record of bonafide work carried out by them under the guidance of **Dr. ASHUTOSH KUMAR DIKSHIT**, Assistant Professor, Department of ECE.

24/5/24

| | |
|---|---|
| **Signature of the guide** | **Signature of Head of the Department** |
| **Dr. Ashutosh Kumar Dikshit**<br>**Assistant Professor** | **Dr. T. Pitchaiah, M.E, Ph.D., MIEEE, FIETE**<br>**Professor & HoD ECE** |

# DECLARATION

We hereby declare that the project report entitled **"SIMULATION AND MODELLING OF SEMICONDUCTOR OPTOELECTRONIC DEVICE(SOLAR CELL)"** is being submitted to Vignan's Foundation for Science, Technology and Research (Deemed to be University) in fulfilment for the award of B.Tech degree in Electronics and Communication Engineering. The work was originally designed and executed by us under the guidance of **Dr. Ashutosh Kumar Dikshit** at Department of Electronics and Communication Engineering, Vignan's Foundation for Science, Technology and Research(Deemed to be University) and was not a duplication of work done by someone else. We hold the responsibility of originality of the work incorporated into this project report.

Signature of the candidates

Harsha Vardhini
Dondeti Harsha Vardhini(201FA05010)

V. Divya.
Vedagiri Divya(201FA05095)

P. Kavya
Palugulla Kavya(211LA05042)

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Name of the Candidates

Dondeti Harsha Vardhini - 201FA05010

Vedagiri Divya - 201FA05095

Palugulla Kavya - 211LA05042

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# ABSTRACT

In current scenario, the energy consumption rate has been increasing day by day. The main source of energy which fulfil our daily energy need is fossil fuels, but problem with these fuels is, they release large amounts of carbon dioxide ($CO_2$), carbon monoxide (CO) or other harmful gases into the atmosphere and leads to global warming.

In addition to that, these types of energy sources are also available in limited amount or finite quantities and cannot be replenished. So, an alternative source of energy is required such as solar energy, wind energy, tidal energy etc. As far as solar energy is concern it directly comes from the sun and contains large amounts of energy and it can be converted directly into electrical energy.

In recent years, metal halide perovskite solar cells (PSCs) have been attractive to researchers due to their increasing power conversion efficiency (PCE). The efficiency of single-junction solar cells was ~3.8 % in 2009and improved significantly by ~25 % in 2020. In this work a Pb-free perovskite solar cell has been designed based on Formamidinium (FA) tin-iodide ($CH_4N_2SnI_3$). The effect of different electron transporting layer (ETL) material on the performance of the solar cell has been studied through substituting the ETL by C60, ZnO, PCBM.

The energy level and charge carrier concentration profiles of the solar cells have been obtained for better understanding the involved mechanisms. The C60 containing solar cell showed the maximum power conversion efficiency($\eta$) of 23.95% at room temperature, with open circuit voltage ($V_{oc}$), short circuit current density ($J_{sc}$) and filling factor (FF) of 1.0233V, 27.066 mA/cm$^2$ and 86.46%, respectively. These results can excite further investigation about the role of ETL in the performance of Pb- free perovskite solar cell.

# Major Design (Final Year Project Work) Experience Information

| | | | |
|---|---|---|---|
| **Student Group** | Dondeti Harsha Vardhini<br>(201FA05010) | Vedagiri Divya<br>(201FA05095) | Palugulla Kavya<br>(211LA05042) |
| **Project Title** | SIMULATION AND MODELLING OF SEMICONDUCTOR OPTOELECTRONIC DEVICE (SOLAR CELL) | | |
| Program Concentration Area | Designing and Optimization of the structure of the solar cell, by which maximum efficiency can be achieved | | |
| **Constraints - Examples** | | | |
| Economic | Fixed budget | | |
| Environmental | Friendly | | |
| Sustainability | Designed to work for long period | | |
| Manufacturability | Yes | | |
| Ethical | Followed the standard professional ethics | | |
| Health and Safety | Guidelines are followed | | |
| Social | Applicable for Household to Industry level | | |
| Political | None | | |
| Other | After finalizing the design of the cell, fabrication of the device can be done | | |
| **Standards** | | | |
| 1.IEEE 255-1963 | IEEE Standard Letter Symbols Semiconductor Devices | | |
| Previous Course Required for the Major Design Experience | 1. Semiconductor Device and Modelling<br>2. Basics of C | | |

**Supervisor**

Arka Bhattacharya
**Project Coordinator**

24/5/24
**Head of the Department ECE**

# LIST OF ACRONYMS AND ABBREVIATIONS

| S.NO | ACRONYMS | ABBREVIATIONS |
|---|---|---|
| 1 | $C_{60}$ | Fullerene |
| 2 | ETL | Electron Transport Layer |
| 3 | eta | Efficiency |
| 4 | FF | Fill Factor |
| 5 | FTO | Fluorine doped Tin Oxide |
| 6 | $FASnI_3$ | Formamidinium Tin Iodide |
| 7 | HTL | Hole Transport Layer |
| 8 | $J_{sc}$ | Short Circuit Current Density |
| 9 | PSC | Perovskite Solar cell |
| 10 | PV | Photo Voltaic Technology |
| 11 | PCBM | Phenyl-$C_{61}$-butyric acid methyl ester |
| 12 | PCE | Power Conversion Efficiency |
| 13 | PEDOT PSS | Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate |
| 14 | SCAPS-1D | Solar Cell Capacitance Simulator-One Dimensional |
| 15 | $V_{oc}$ | Open Circuit Voltage |
| 16 | ZnO | Zinc Oxide |

# CHAPTER 1

# INTRODUCTION

## 1.1 History

The daily activities of human civilization consume a vast quantity of energy. We rely heavily on fossil fuels (oil, coal, and gas) to supply this energy need. Non-renewable resources are typically transformed into electrical energy to produce various forms of energy. Furthermore, this type of energy is well-suited to energy transmission, distribution, and control, and as a result, even energy shortages in remote rural areas can be easily alleviated. Energy consumption is critical to every country's development, and a country's literacy rate is closely related to its per capita energy consumption. As a result, the development of developing countries needs a massive amount of energy.

Because making this much safe and sustainable energy available is a major issue for humanity. It must also be ecologically friendly and economically viable for all industries. As a result, fossil fuels are unlikely to be our most promising candidate. From an economic standpoint, the worrisome rise in the price of fossil fuels (petrol, diesel, and kerosene) is a big worry. Similarly, as a result of the usage of fossil fuels, greenhouse gas emissions and their negative impacts on the environment, such as global warming, have become a major concern. The interconnected global warming and pollution issues with power generation facilities, such as hydroelectric and thermal power, pose genuine hazards to society. As a result, we must work together to play with ecology and sustainable development in order to achieve a green environment.

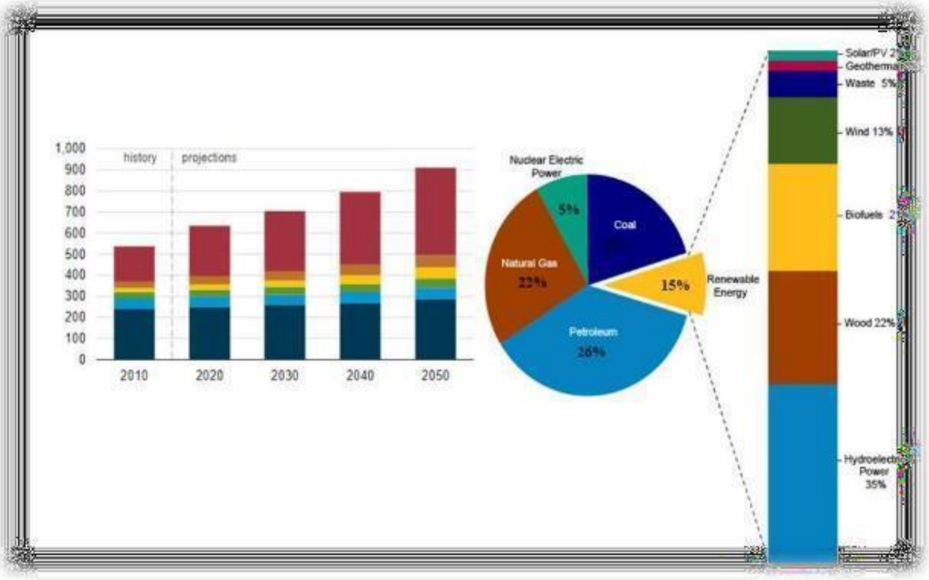

Figure 1.1: World energy demand and energy contributions from various energy resources

Non-renewable energy resources account for around 85% of overall energy use (Figure 1.1), and they will soon be consumed due to the limited availability of essential resources on the planet. Furthermore, the different poisonous gases and by-products produced as a result of the use of renewable energy sources pose a slew of major issues for humanity, including global warming, respiratory disorders, and so on.

These negative consequences will only get worse in the future, affecting our future generations. As a result, it is the time to concentrate on developing new renewable energy sources to meet the increased energy demand. Various renewable and non-renewable energy resources are available in the midst of the urgent energy crisis, and these are expected to meet such vitality needs. According to the International Energy Outlook 2019, global energy consumption will reach 911 quadrillion by 2050. (BTU). Wind energy, solar energy, thermal energy, tidal energy,and other renewable energy technologies area available to meet our energy requirements. The contribution of renewable energy sources is illustrated in Figure 1.2, which shows the six predicted applications of these approaches.

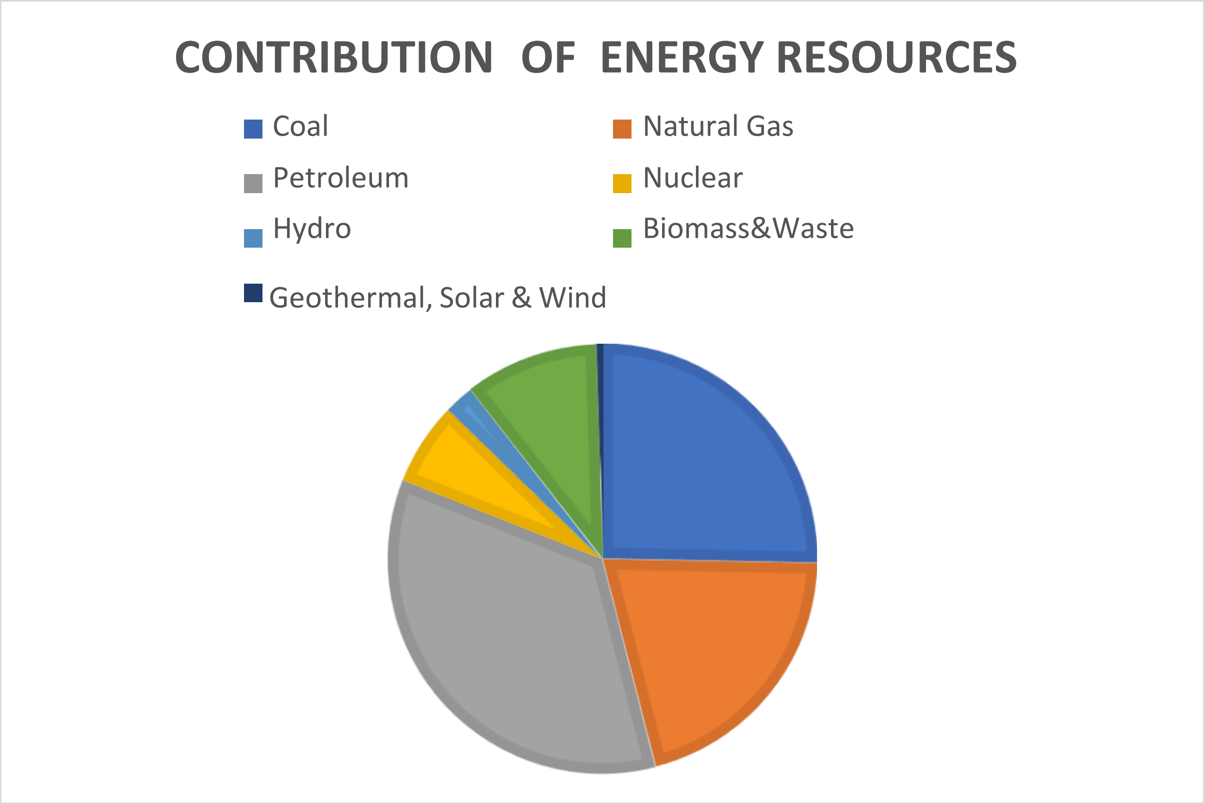

Figure 1.2: Contribution of non-renewable and renewable energy sources

The share of renewable energy is increasing, whilst fossil fuel usage is decreasing year after year, as seen in Figure 1.2. There are various types of renewable energies technologies are available which meet out energy requirement such as wind energy, solar energy, thermal energy, tidal energy etc. The projected utilization of these techniques is, depicted in the Figure 1.3, indicating the contribution of renewable energy sources. Solar energy-based power generation is the fastest-growing renewable source among the various options.

Solar power generators have several advantages over other renewable energy sources, includingsimplicity of energy gathering, inexpensive installation costs, and greater reliability. It is predicted that the energy harvested by the sun will be sufficient to meet our energy needs. We can reduce the harmful effects of energy production on the environment by avoiding the use offossil fuels. Given the negative effects of fossil fuels and the potential benefits of solar-based devices, most governments prioritize the installation of photovoltaic devices in order to save the environment globally.

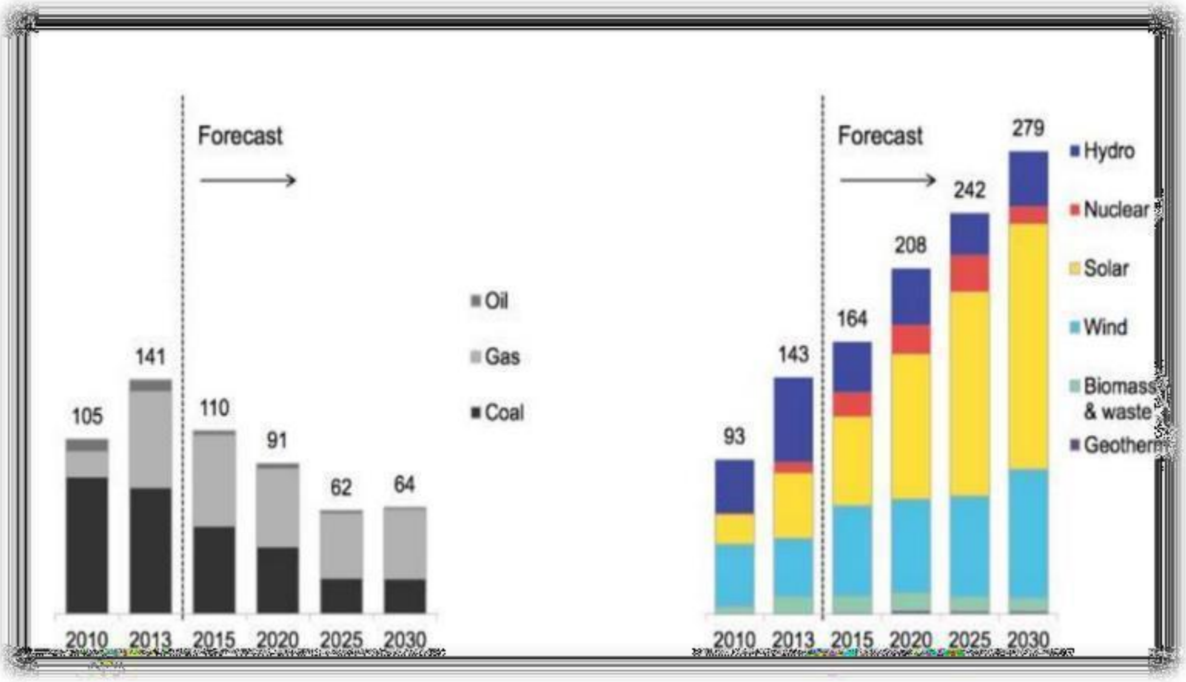

Figure 1.3: Contribution of various energy resources in generation of electricity [2]

In 2018, solar power stations with capacity around 512.3 GW were installed with ~25% growthrate. These installations were made by international energy agency of photovoltaics power system programme (IEA-PVPS) countries and non-IEA- PVPS countries with contribution 432.7 GW and 79.6 GW respectively.

The comparison of India’s position with global scenario, regarding installation and harvesting the solar energy, India stood at 2nd position with installation of power stations with capacity 10.8 GW, in 2018. In Asia, China is able to installedSolar powered stations of capacity 175.4 GW; and American continent north America installed
10.7 GW capacity solar stations in 2018 [3].

A pictorial representation of worldwide production capacity of solar energy is depicted in Figure 1.4. The accompanying segment gives a concise overview regarding the development of the solar energy or photovoltaic innovation over the years.

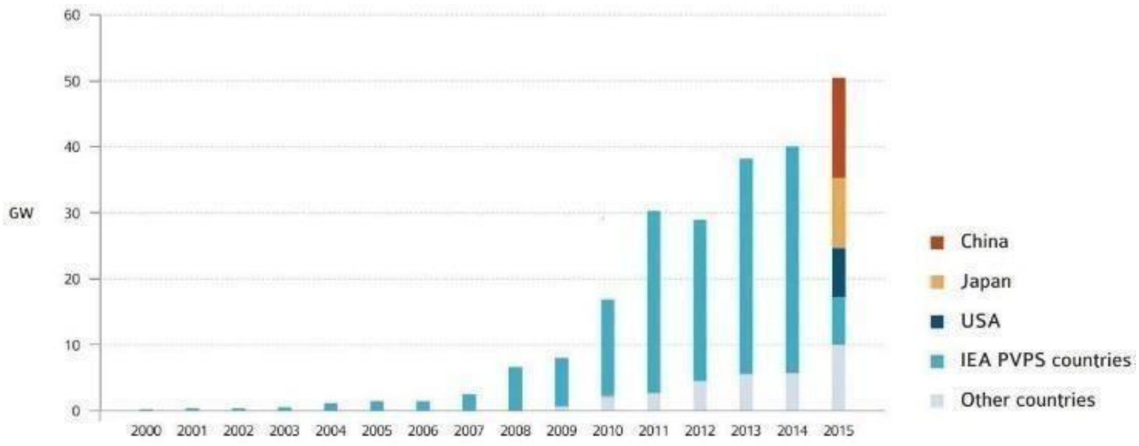

Figure 1.4: Development of PV generation capacity by IEA and non-IEA PVPS countries [3].

As of October 2022, India's installed renewable energy capacity (including hydro) stood at

165.94 GW, representing 40.6% of the overall installed power capacity. The country istargeting about 450 Gigawatt (GW) of installed renewable energy capacity by 2030 – about 280GW (over 60%) is expected from solar.

The non-hydro renewable energy capacity addition stood at 4.2 GW for the first three months ofFY23 against 2.6 GW for the first three months of FY22.Solar power installed capacity has increased by more than 18 times, from 2.63 GW in March 2014 to 49.3 GW at the end of 2021. In 2022, till November, India has added 12 GW of solar power capacity. Power generation from renewable energy sources (not including hydro) stood at 16.18 billion units (BU) in September 2022, up from 14.49 BU in September2021.With a potential capacity of 363 GW and with policies focused on the renewable energy sector, Northern India is expected to become the hub for renewable energy in India.

# CHAPTER 2

# SOLAR CELL

## 2.1 Evolution of Solar Cell

A solar photovoltaic cell, also known as a solar cell, is a semiconductor-based device that converts incident solar radiation into electrical energy. After the discovery of the photovoltaic effect, which states that when semiconductor material is exposed to sunlight, voltage develops, research in the field of solar cells has progressed. In 1839, French physicist Edmond Becquerel hypothesised this phenomenon for the first time [4].

The photovoltaic effect was first seen in an electrolytic cell, which consists of two platinum electrodes coated with silver chloride and immersed in an acidic liquid, generating voltage and current when exposed to sunshine. Willoughby Smith noticed a comparable effect in the selenium element after more than 30 years of such reporting [5].

Charles Fritts invented the first solar cell in 1894, which had a 1% efficiency. Of course, such a low efficiency cell is unsuitable for use in practical devices. In 1954, three Bell Labs USA scientists, Pearson, Chapin, and Fuller, produced a p-n junction- based solar cell with an efficiency of > 4% [6,7].

This finding was a watershed moment in photovoltaics. The currently developed cell uses lithium as a doping element for forming junctions, however this is changed with boron doping, which increases the cell's efficiency from 4% to 6% [8].

The current silicon solar cell technology is following the path established by this finding. Silicon solar cell efficiency improved with the introduction of silicon technology. The efficiency of the Silicon solar cell improved to 14 percent in the 1970s, and solar cells were quickly used for space missions [9,10].

Later, due to the relentless efforts of academic institutes and research laboratories, substantial advancements in solar technology were documented. Overall, a 400 time increase in efficiency has been obtained. Amorphous silicon (a-Si), Cadmium Telluride (CdTe), Cadmium Sulphide (CdS), Gallium Indium Phosphide (GaInP), organic, inorganic, organic-inorganic hybrid, perovskite, and other materials have all been investigated in solar cell research [11-18].

These materials are proposed as a possible alternative to silicon and are thoroughly investigated. These materials are utilized to create improved solar cells. The material used determines the constructed devices' stability,cost, and conversion efficiency.

## 2.2 Generations of Solar Cell

Numerous solar cells have been developed and classed during the last 70-80 years based on the active or absorbent material used in their construction. A solar cell can be classified into three main categories, as shown in the flow chart (Figure 2.1).

### 2.2.1 First Generation

The first-generation solar cell is a semiconductor solar cell made from c-Si/III-V group semiconductors. The type of solar cells is determined by the nature of active material, such as silicon, gallium arsenide (GaAs), indium phosphide (InP), and others. It is further divided into two types: single junction and multi-junction solar cells.

Only one type of absorbing material, such as GaAs/InP or mono/multi c-Si, and one p-n junction are employed in a single junction. In a single junction solar cell, the p and n layers are usually made of the same material, however in a multi-junction solar cell, one or more semiconductor (p-n) junctions are combined with other active absorbing materials.

To aid charge flow, these various active absorbing materials are placed in decreasing bandgap order from top to bottom. Mono and multi-junction Si solar cells, as well as InP/GaAs solar cells, are examples of single-junction first-generation solar cells, whereas multi-junction solar cells include GaInAsP/GaIn (double junction), GaInP/GaAs(doublejunction),GaInP/GaAs/InGaAs(triplejunction),GaInP/GaAs/GaInAs4r/GaIn (four junction),etc.

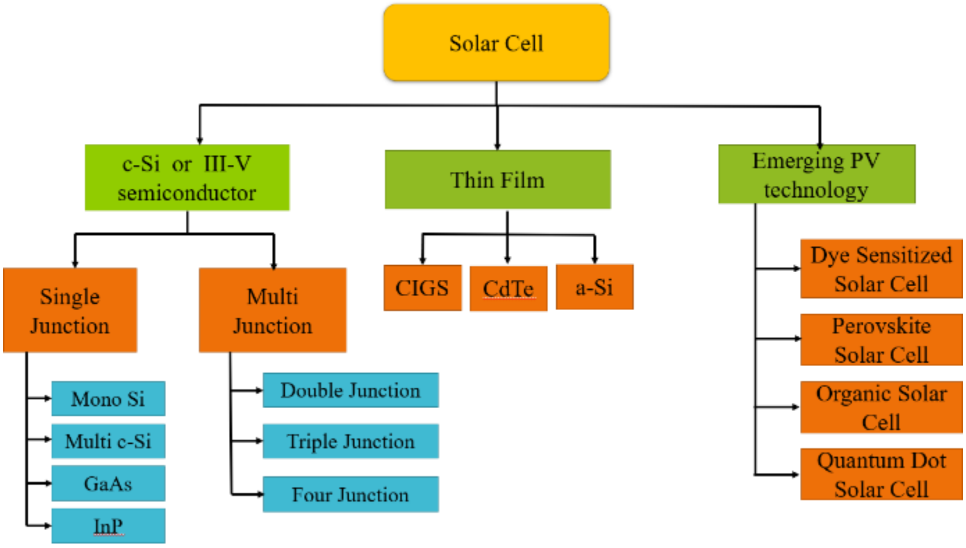

Figure 2.2.1: Schematic of classification of solar cell

### 2.2.2 Second Generation

Thin-film solar cells, often known as second-generation solar cells, are a distinct category of solar cells. The active material thickness in this sort of cell is a few microns, and the p-n junction is made of the same materials as the active material. If both the p-type and n-type materials are the same, the device is called homojunction; if the materials are different, the device is called heterojunction. Copper Indium Gallium Selenide (CIGS), Cadmium Telluride (CdTe), and hydrogenated amorphous silicon (a-Si:H) are examples of second-generation solar cells.

### 2.2.3 Third Generation

The third generation of solar cell technology includes the upcoming PV technology. Dye-sensitized solar cells, perovskite solar cells, quantum dot (QD) solar cells, organic solar cells, and others are examples of the third generation of solar cells. Ruthenium poly pyridine dye, PCBM, P3HT, or their mixes are preferred active ingredients in dye-sensitized solar cells. Nano-sized materials such as PbS,CdTe, and others are employed as absorbing materials in quantum dot solar cells [19-22]. Materials such as methyl ammonium lead trihalide ($CH_3NH_3PbX_3$) (X=halogen) are used in perovskite solar cells [23].

## 2.3 Photovoltaics process in solar cell

To convert solar energy into electric energy, the total solar cell functioning incorporates crucial optical and electrical processes. The following are the key background processes:

i. Solar photon absorption.
ii. Charge generation.
iii. Charge separation.
iv. Charge transportation.

### 2.3.1 Solar Photon Absorption

When a solar photon impinges on the upper active layer of the solar cell, it may get absorbed and induce electron from the valence band (VB) of layer material to move in the conduction band (CB). This electronic transition (VB to CB) is subject to the adequate photon energy $h\upsilon > Eg$ (wavelength $\lambda < hc/Eg$) required to produce free electrons and holes. The photon absorption is quantified by the universal parameter absorption coefficient "$\alpha$". Absorption coefficient estimate by the following relation:

$$N_t = N_0 \exp(-\alpha x) \qquad (1)$$

where $N_t$ and $N_0$ is the number of photons at the given time after and before the light incidence, respectively. The term "$x$" represents the path length in the semiconductor.

Further, with the reduction in path length or thickness of the wafer, photon absorption reduces. One should wisely select the semiconductor element having a bandgap comparable to the incident photon energy. To utilize a full working solar spectrum, absorbent material should possess a significant extinction coefficient (0.0189 for c-Si), in addition to that, it may have a small bandgap (~1.1eV for Si) and appropriate Fermi level position.

### 2.3.2 Charge Generation

The photon absorption leads a generation of electron-hole pairs (EHPs), and the rate ofEHP generation per unit volume per unit time $G(x)$ is given as:

$$G(x) = -\frac{\mathrm{dNph}}{\mathrm{dx}} = \alpha N_0 \exp(-\alpha x) \qquad (2)$$

### 2.3.3 Charge Separation

The subsequent event after generating electron-hole pair is the extraction of charges immediately before they recombine. Recombine may avoid by creating asymmetry in the structure. The charge separation may be accomplished by an electric field that drifts electrons and holes into the opposite directions. The better dissociation of charge carrier (electron and hole) in the opposite direction may achieve by effective arrangement of band structure and proper alignment of Fermi level.

### 2.3.4 Charge Transportation

Transportation of charge-carrier to the contact electrodes is a very crucial process. The adequate charge carrier transportation to the contact is subject to high carrier lifetime (τ), considerable diffusion length ($L_d$), high mobility (μ), etc. For that purpose, proper selection of electrodes is necessary.

## 2.4 Solar Cell Parameters

### 2.4.1 Short-Circuit Current (Jsc)

This current is the maximum current attain by the solar cell when its terminals are short-circuited. Factor $J_{SC}$ depends upon the semiconductor (SC) bandgap expressed by the following relation:

$$J_{SC} \alpha \frac{1}{Band\ gap\ of\ SC} \tag{3}$$

Numerically, $J_{SC}$ is calculated by integrating the photon flux within a limit of the highest photon energy to the cut-off energy level (bandgap of the SC) and multiplied by elementary charge q ($1.6 \times 10^{+19}$ C).

### 2.4.2 Open-Circuit Voltage (Voc)

Open-circuit voltage is the maximum voltage obtains across the solar cell when its terminals are open. The open-circuit voltage, $V_{OC}$ is decided by the semiconductor bandgap, and the upper limit of the $V_{oc}$ is equivalent to the semiconductor bandgap. Further, $V_{oc}$ indicatesthe potential level difference of the contacts (quasi-Fermi level of the SC), which sets the upperlimit of the $V_{oc}$ of the solar cell. Mathematically, it is expressed by the following relation

$$V_{OC} = \frac{KT}{q} \ln\left(\frac{I_L}{I_0} + 1\right) \tag{4}$$

where, $I_L$ and $I_0$ are the load current and the recombination current, respectively. The high $V_{oc}$can be achieved by the keeping $I_0$ small.

### 2.4.3 Efficiency(η)

The efficiency of a solar cell is defined as its ability to convert the solar photon into electricityand is expressed as follows

$$\eta = \frac{V_{oc} I_{sc}(FF)}{P_{.}} \qquad (5)$$

Where, $V_{oc}$ is the open circuit voltage, $J_{sc}$ is short circuit current, FF is filling factor of the celland $P_d$ is solar photon density coming from the sun.

### 2.4.4 Fill Factor (FF)

The fill factor depends upon the value of series and shunt resistances of the solar cell. Series resistance comprises the emitter, base, and metal-semiconductor contact resistances that occur in the path of the cell. The shunt resistance is due to the leakage across the p-n junction, and it includes the periphery of the device, crystal defects, and impurities at the intersection. For an efficient solar cell, series resistance should be low, whereas shunt resistance should be high. The fill-factor is given by

$$FF = \frac{v_{oc} - \ln(v_{oc} + 0.72)}{v_{oc} + 1} \qquad (6)$$

where $v_{oc}$ is ${V_{oc}}/{(kT/q)}$

### 2.4.5 Principle of Solar Cell

A solar cell is a device that **directly converts the energy of light into electrical energy through the photovoltaic effect**. Solar cells or photovoltaic cells are made based on the principle of the photovoltaic effect. They convert sunlight into direct current (DC) electricity.

# CHAPTER 3

# PEROVSKITE SOLAR CELL

A perovskite is any material with a crystal structure following the formula $ABX_3$, which was first discovered as the mineral called perovskite, which consists of calcium titanium oxide ($CaTiO_3$). The basic structure of a perovskite solar cell consists of an electron transporting layer (ETL) and a hole transporting layer (HTL), where the free electrons and holes get injected into. Usually, the anode and cathode in the perovskite solar cell structure are formed by Indium-doped tin oxide (ITO) glass and metal.

Solar cells made with perovskites work in a similar fashion to traditional solar panels – a semiconductor absorbs solar energy and initiates a flow of electrons, which is captured by wiring and converted into usable electricity.

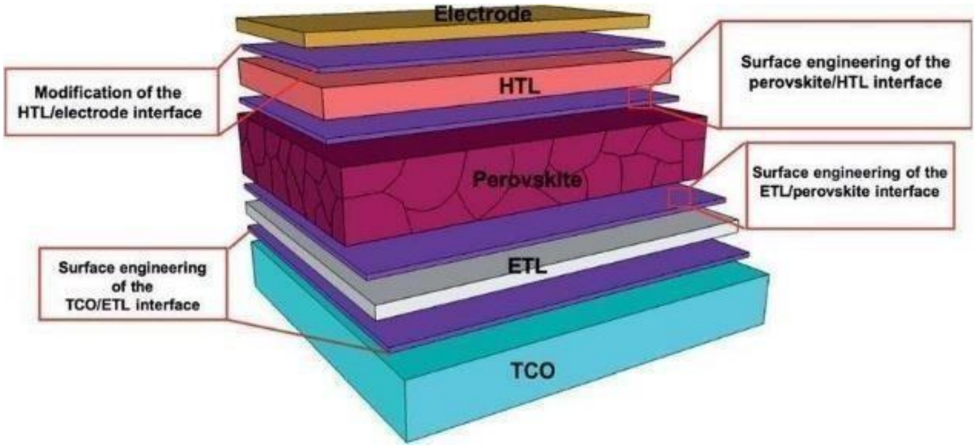

Fig 3.1: Different layers of a Perovskite Solar Cell [23]

### 3.1 Stability and Durability

Perovskite solar cells have demonstrated competitive power conversion efficiencies (PCE) with potential for higher performance, but their stability is limited compared to leading Photovoltaic(PV) technologies. Perovskites can decompose when they react with moisture and oxygen or when they spend extended time exposed to light, heat, or applied voltage.

To increase stability, researchers are studying degradation in both the perovskite material itself and the surrounding device layers. Improved cell durability is critical for the development of commercial perovskite solar products.

Despite significant progress in understanding the stability and degradation of perovskite solar cells, they are not currently commercially viable because of their limited operational lifetimes,Commercial applications outside the power sector may tolerate a shorter operational life, but even these would require improvements in factors such as device stability during storage. For mainstream solar power generation, technologies that cannot operate for more than two decades are unlikely to succeed, regardless of other benefits.

Early perovskite devices degraded rapidly, becoming non-functional within minutes or hours. Now, multiple research groups have demonstrated lifetimes of several months of operation. For commercial, grid-level electricity production, SETO is targeting an operational lifetime of at least 20 years, and preferably more than 30 years.

The perovskite PV research and development (R&D) community is heavily focused on operational lifetime and is considering multiple approaches to understand and improve stability and degradation. Efforts include improved treatments to decrease the reactivity of the perovskite surface, alternative materials and formulations for perovskite materials, alternative surrounding device layers and electrical contacts, advanced encapsulation materials, and approaches that mitigate degradation sources during fabrication and operation.

One issue with assessing degradation in perovskites is developing consistent testing and validation methods. Research groups report performance results based on highly varied test conditions, including different encapsulation approaches, atmospheric compositions, illumination, electrical bias, and other parameters. While such varied test conditions can provide insights and valuable data, the lack of standardization makes it challenging to directly compare results and difficult to predict field performance from test results.

### 3.2 Power Conversion Efficiency

In small-area lab devices, perovskite PV cells have exceeded almost all thin-film technologies (except III-V technology) in power conversion efficiency, showing rapid improvements over the past five years. However, high-efficiency devices have not necessarily been stable or possible to fabricate at large scale. For widespread deployment of perovskites, maintaining these high efficiencies while achieving stability in large-area modules will be necessary. Continued improvement in efficiency in medium-area modules could be valuable for mobile, disaster response, or operational energy markets where lightweight, high-power devices are critical.

### 3.3 Working of Perovskite Solar Cell

The perovskite solar cell works as a pin diode with the active absorber perovskite layer acts asan intrinsic semiconductor layer, the Hole transport layer acts as the $P^+$ layer and the electron transport layer acts as the $N^+$ layer. The metallization layers act as electrical accessing electrodes. when the device is illuminated the photons penetrate to the active layer where there will be generation of electron hole pairs. These electron hole pairs will be separated by the electric field the electrons will move to the ETL and the holes will move to the HTL. Finally, they reach the corresponding electrode.

# CHAPTER 4

## SOFTWARE

SCAPS is a one-dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium. SCAPS is originally developed for cell structures of the CuInSe2 and the CdTe family. Several extensions however have improved its capabilities so that it is also applicable to crystalline solar cells (Si and GaAs family) and amorphous cells (a-Si and microporous Si). An overview of its main features is given below:

- We can add up to 7 semiconductor layers

- Almost all parameters can be graded (i.e., dependent on the ocal composition or on the depth in the cell): Eg, χ, ε, NC, NV, Vthn, Vthp, μn, μp, NA, ND, all traps (defects) Nt

- Recombination mechanisms: band-to-band (direct), Auger, SRH-type

- Defect levels: in bulk or at interface; their charge state and recombination is accounted for

- Defect levels, charge type: no charge (idealization), monovalent (single donor, acceptor), divalent (double donor, double acceptor, amphoteric), multivalent (user defined)

- Defect levels, energetic distributions: single level, uniform, Gauss, tail, or combinations

- Defect levels, optical property: direct excitation with light possible (impurity photovoltaic effect, IPV)

- Defect levels, metastable transitions between defects

- Contacts: work function or flat-band; optical property (reflection of transmission filter) filter

- Tunnelling: intra-band tunnelling (within a conduction band or within a valence band); tunnelling to and from interface states

- Generation: either from internal calculation or from user supplied g(x) file

- Illumination: a variety of standard and other spectra included (AM0, AM1.5D, AM1.5G, AM1.5Gedition2, monochromatic, white...) illumination: from either the p-side or the n-side; spectrum cut-off and attenuation

- Working point for calculations: voltage, frequency, temperature

- The program calculates energy bands, concentrations and currents at a given working point, J-V characteristics, ac characteristics (C and G as function of V and/or f ), spectral response (also with bias light or voltage)

- Batch calculations possible; presentation of results and settings as a function of batch parameters

- Loading and saving of all settings; start-up of SCAPS in a personalized configuration; a script language including a free user function

- Very intuitive user interface

- A script language facility to run SCAPS from a ‘script file’; all internal variables can be accessed and plotted via the script.

- A built-in curve fitting facility

- A panel for the interpretation of admittance measurements

**Procedure:**

1. Run SCAPS-1D
2. Define the problem, thus the geometry, the materials, all properties of your solar cell.
3. Indicate the circumstances in which you want to do the simulation, i.e. specify the working point.
4. Indicate what you will calculate, i.e. which measurement you will simulate.
5. Start the calculation(s).
6. Display the simulated curves.

**Run SCAPS:**

Double-click the file scaps3200.exe in the file manager (or any other SCAPS version). SCAPS opens with the Action Panel.

**Define the problem:**

Click the button set problem in the action panel, and chose load in the lower right corner of the panel that opens. Select and open e.g. the file NUMOS CIGS baseline.def: that is the example problem file of the practicum session at the NUMOS workshop, Gent, 30 march 2007. This file is supposed to be in the folder /SCAPS/def, where /SCAPS/ stands for the directory whereyou installed SCAPS, and where the SCAPS .exe file resides. If necessary, browse to find this file in a later stage, you can alter all properties of the cell by clicking set problem in the actionpanel.

**Define the working point:**

The working point specifies the parameters which are not varied in a measurement simulation and which are relevant to that measurement. Thus:

- The temperature T: relevant for all measurements. Note: in SCAPS, only $N_C(T)$, $N_V(T)$, the thermal velocities, the thermal voltage kT and all their derivatives are the only variables which have an explicit temperature dependence; you must input for each T the corresponding materials parameters yourself.

- The voltage V: is discarded in I-V and C-V simulation. It is the dc-bias voltage in C-f simulation and in QE (λ) simulation. SCAPS always starts at 0 V, and proceeds at the working point voltage in a number of steps that you also should specify.

- The frequency f: is discarded in I-V, QE (λ) and C-f simulation. It is the frequency at which the C-V measurement is simulated.

- The illumination: is used for all measurements. For the QE (λ) measurement, it determines the bias light conditions. The basis settings are: dark or light, choice of the illuminated side, choice of the spectrum. A 1 sun (= 1000 W/m2) illumination with the 'air mass 1.5, global' spectrum is the default, but you have a large choice of monochromatic light and spectra for your specialized simulations. If you have an optical simulator at your disposal, you can immediately load a generation profile as well instead of using a spectrum.

**Select the measurement(s) to simulate:**

In the action-part of the Action Panel, you can select one or more of the following measurements to simulate: I-V, C-V, C-f and QE (λ). Adjust if necessary, the start and end values of the argument, and the number of steps. Initially, do one simulation at a time, and use rather coarse steps: your computer and/or the SCAPS program might be less fast than you hope, or your problem could be really tough.

**Start the calculation(s):**

Click the button calculate: single shot in the action panel. The Energy Bands Panel opens, andthe calculations start. At the bottom of the Panel, you see a status line, e.g. "iv from 0.000 to 0.800 Volt: V = 0.550 Volt", showing you how the simulation proceeds. Meanwhile, SCAPS stands you a free movie how the conduction and valence bands, the Fermi levels and the whole caboodle are evolving.

### Display the simulated curves:

After the calculation(s), SCAPS switches to the Energy band panel (or the AC-band panel). You can now look at your ease to the band diagrams, carrier densities, current densities, at the last bias point calculated (stop your calculations earlier, or use the pause button on the Action Panel if you want to look at an intermediate state at ease). You can output the results (buttons print, save graphs, show (then the numbers are shown on screen; cut & paste to e.g. Excel is possible), or save (then the numbers are saved to a file). You can switch to one of the specialized output Panels (if you have already simulated at least one corresponding measurement). We only show the example of the IV Panel.

### Editing the problem:

Go to the Action Panel, click set problem. You are now in the Solar Cell Definition Panel. Clickon a layer name, and you enter the Layer Properties Panel where you can change all parametersof that layer. Use your intuition and/or read the rest of this manual.

### Speeding up: Batch calculations

When you want to explore the influence of one or a few parameters to the solar cell characteristics, you can take profit of the batch option. When you click Batch set-up, a panel opens where you can choose which parameter to vary, over which range, and in which mode (Lin, Log or custom). You can also define more than one parameter, and vary all of them (in a nested way or ‘simultaneous’), but be modest to start. A batch calculation is launched when calculate: batch is clicked.

**Speeding up: Recorder:**

In a regular single shot or batch calculation, the detailed panels are only available for the last measurement point. To be able to see them as a function of the batch parameters you can launch a record calculation. You should first select the properties which you want to keep track of by clicking Record set-up. Browse through the property-lists, and don’t forget to press one of the insert buttons to add a property to the recorder list. By clicking calculate: recorder, a recorder calculation is launched. Cell parameters are varied according to the Batch set-up, and all simulations are performed which are needed to determine the asked properties. This means the selected measurements on the action panel are ignored.

# CHAPTER 5

## DEVICE STRUCTURE AND SIMULATION

The active layer in the PSC is mainly $CH_3NH_3PbI_3$ because of its greater absorbing nature of the sunlight and the solar cells with $CH_3NH_3PbI_3$ as the absorber material exhibits higher efficiency. But the lead component in this causes a huge environmental damage and it is health hazardous too. So it is better to look for an alternative which is lead free i.e, $CH_4N_2SnI_3$.This can also be used as an active layer in PSCs and it is not a hazardous material since the absence of the lead. But the efficiency of the solar cell which uses $CH_3NH_3SnI_3$ as active material exhibits less efficiency than the solar cells with $CH_3NH_3PbI_3$ as the active material.

In order to improve the efficiency of Pb-free based PSC there is a need to search for different combinations of ETL materials to get the considerable efficiency. We simulated the solar cell with C60, PCBM, ZnO. We achieved a higher efficiency of 23.95% with C60 as ETL.This Semiconductor Solar cell design as per the IEEE Standard 255-1963.

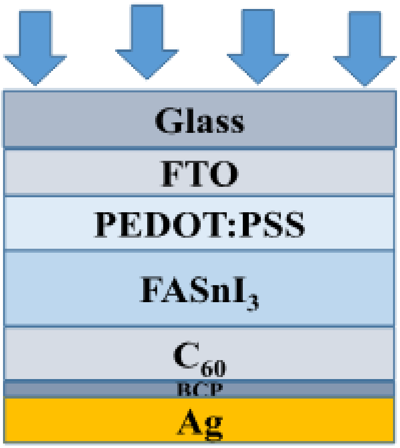

Figure 5: Device structure of perovskite solar cell

## 5.1 RESULTS AND DISCUSSION :

In order to get the efficient structure for the lead-free perovskite solar, optimization of the layer has been done for the ETL, HTL as well as absorber layer. In addition to that defect density between the ETL/Active material as well as HTL/ Active material is varied and performance of the device is investigated. The observation are as follows:

### A. Influence of Thickness of ETLs

Electron transport layer (ETL) plays a very crucial role in order to calculate the overall efficiency of the cell and it is calculated by changing the different ETLs like C60, ZnO, PCBM by fixing the thickness of the absorber layer and HTL layer i.e. 350 nm and 50 nm respectively. It is clearly observed from the Figure 6.1 there is no significant change in efficiency was observed by varying the thickness of the layer. So, by keeping fabrication limitations and other parameters of the cell, 50nm thin layer is the optimized thickness for ourstructure. Max Eff - 26.95%(C60).

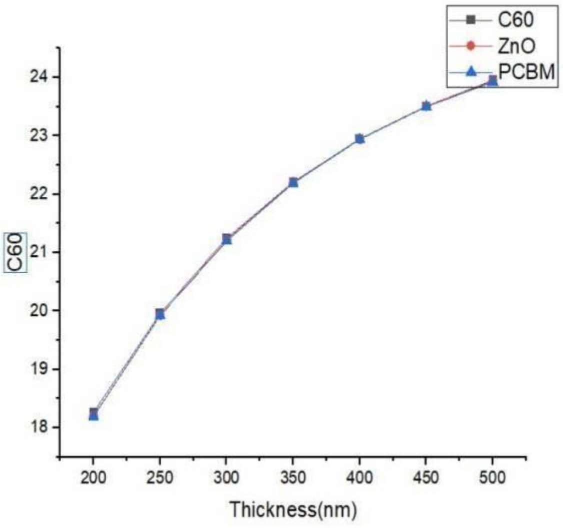

Figure 5.1.1: Effect of thickness of ETLs

### B. Influence of Thickness of Absorber layer

One of the most important factors in optimizing solar cell performance is the active layer thickness. It should be chosen with care to increase current density while keeping the reverse saturation current to a minimum. Due to increasing series resistance and internal power loss in a larger absorber layer, FF is inversely proportional to perovskite thickness. The increase in the dark saturation current, which promotes charge carrier recombination, is responsible for the drop in $V_{oc}$ as thickness increases.

This is explained by the relationship between open-circuit voltage and photo-generated currentand dark saturation current. For the thickness of **300nm** of absorber layer we got the best performance of the cell with PCE of 21.25%. Now we will optimize the thickness of the absorber layer of this cell to obtain better performance. We got a PCE value of 23.95% which is increased by 2.88%, FF of 86.46%, $V_{oc}$ of 1.0233, and $J_{sc}$ of 27.066920mA/cm^2 when we makethe thickness of the absorber layer 1000nm.

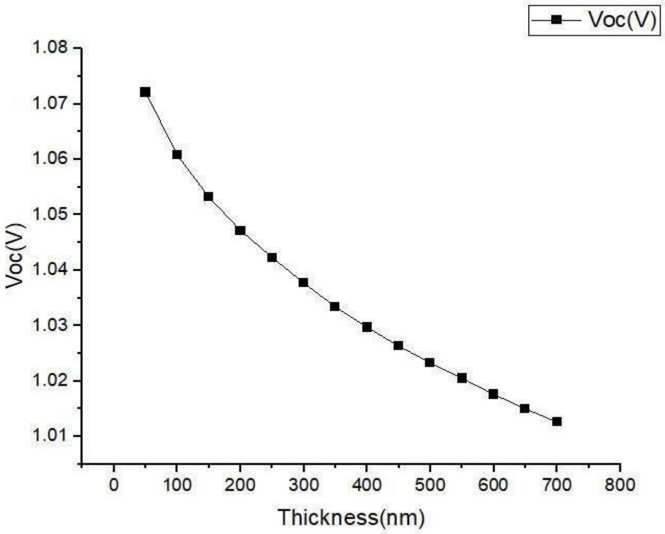

Figure 5.1.2: Effect of Thickness of FASnI3 onVoc(V)

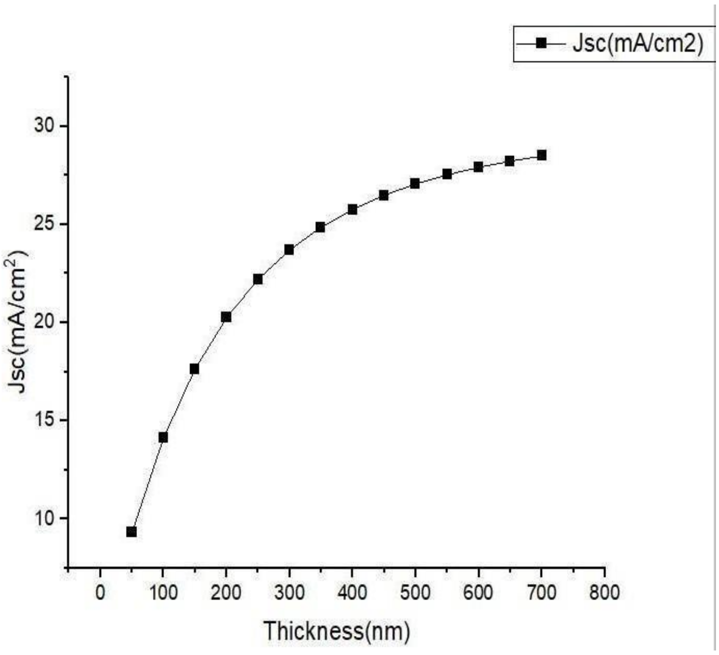

Figure 5.1.3: Effect of Thickness of FASnI3 on $J_{sc}$(mA/cm$^2$)

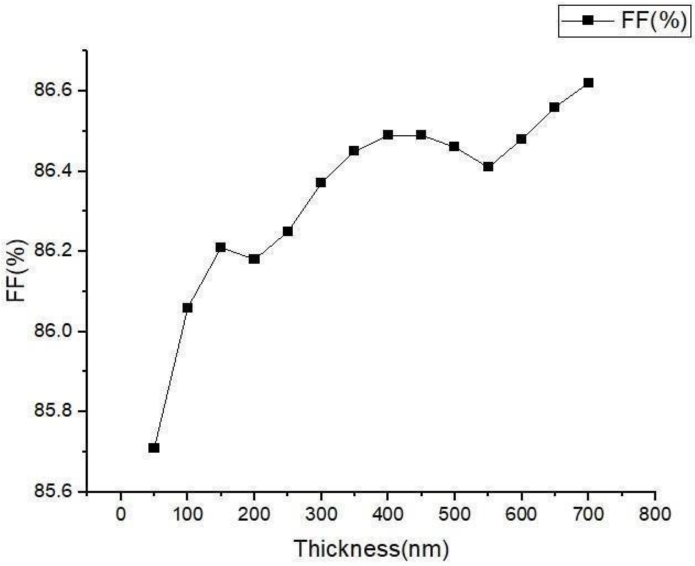

Figure 5.1.4: Effect of Thickness of FASnI3 on FF(%)

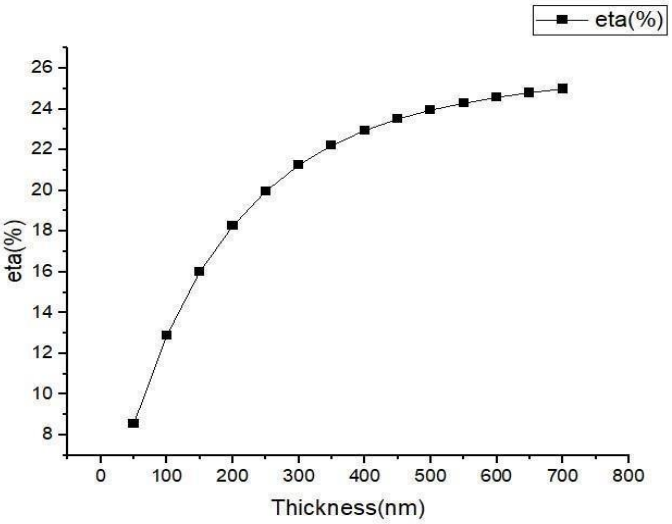

Figure 5.1.5: Effect of thickness of FASnI3 on eta(%)

## C. Influence of Defect Density of the Absorber layer

The total defect density of the active layer is another critical characteristic that can have a major impact on device performance. Higher defect concentrations in the absorber layer result in increased recombination due to the formation of pinholes, a faster rate of film deterioration, less stability, and lower overall device performance.

The simulation was done by varying the total defect density from $1 \times 10^{13}$cm$^{-3}$ to $1 \times 10^{17}$ cm$^{-3.}$ When the total defect density in the absorber layer is raised, all cell performance suffers. The defect density has a significant impact on FF, which is a critical parameter impacting the cell's efficiency. At a defect density of 1x$10^{17}$cm3, FF can be as low as 49.87 percent.

Furthermore, as the defect density grows from 1x$10^{13}$cm$^{3}$ to 1x$10^{17}$ cm$^{3}$, the efficiency drops dramatically from 25.87 percent to 10.49 percent. We infer that defect density has a direct impact on efficiency because increased defects result in a reduction in charge carrier diffusion length and the addition of recombination carriers in the absorber layer.

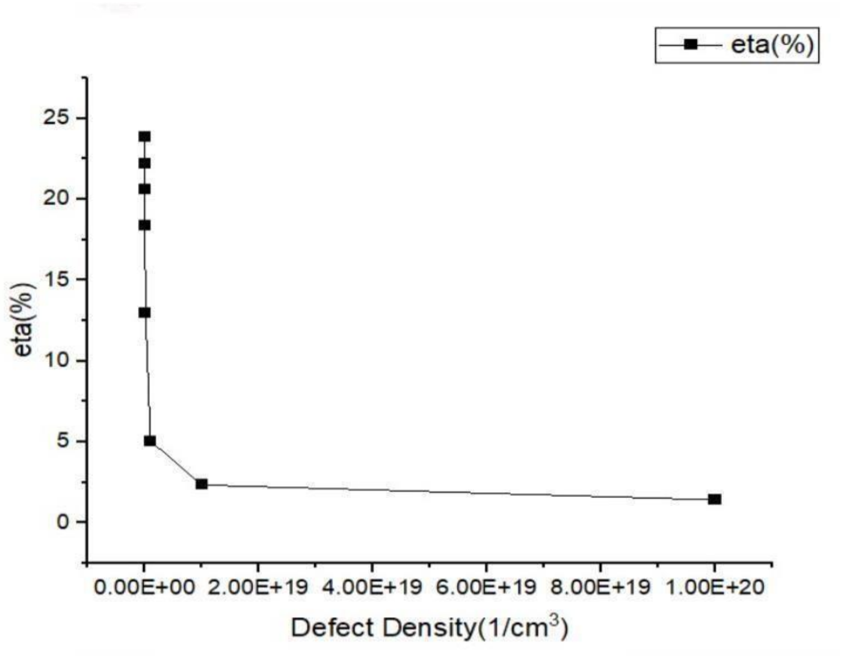

Figure 5.1.6: Effect of Defect Density(1/cm$^3$) of FASnI3 on eta(%)

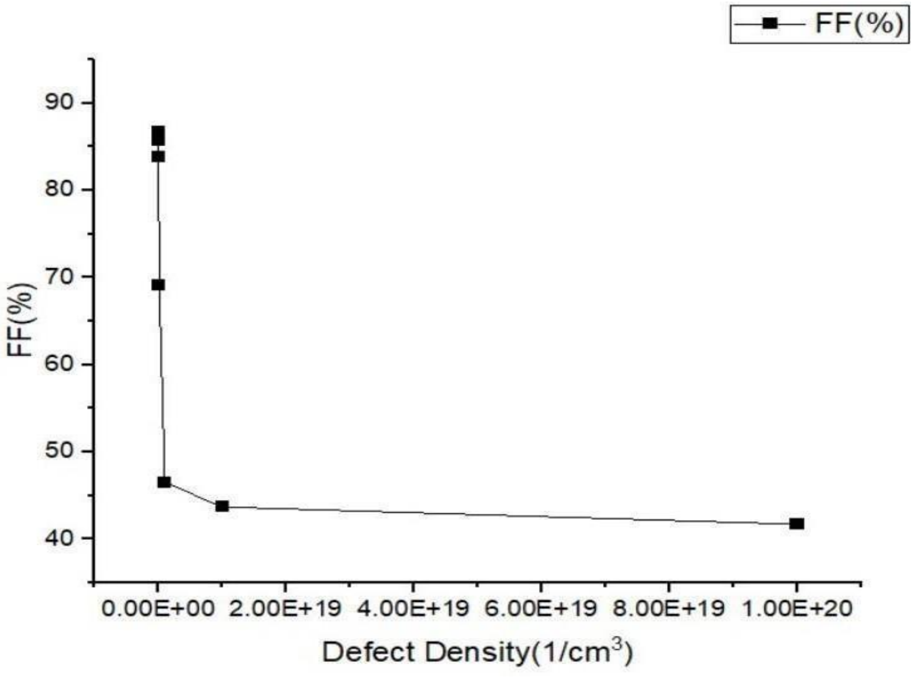

Figure 5.1.7: Effect of Defect Density(1/cm$^3$)of FASnI3 on FF(%)

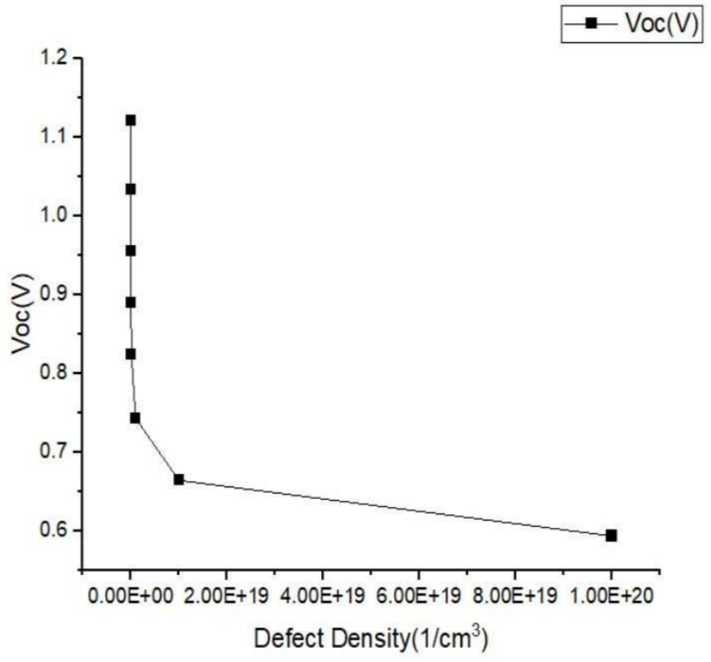

Figure 5.1.8: Effect of Defect Density(1/cm$^3$) of FASnI3 on $V_{OC}$(V)

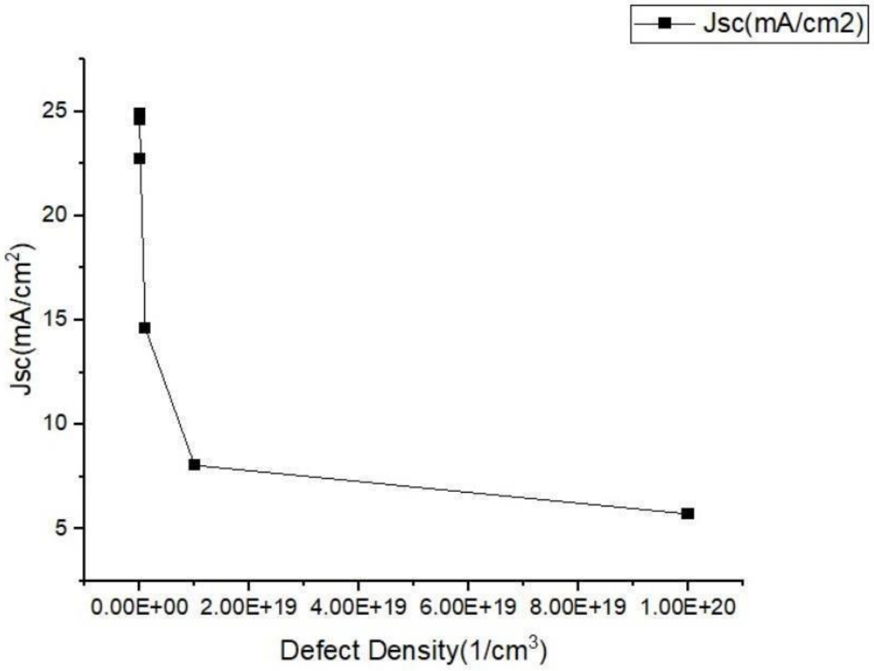

Figure 5.1.9: Effect of Defect Density(1/cm$^3$) of FASnI3 on $J_{SC}$(mA/cm$^2$)

### D. Influence of Temperature on Solarcell

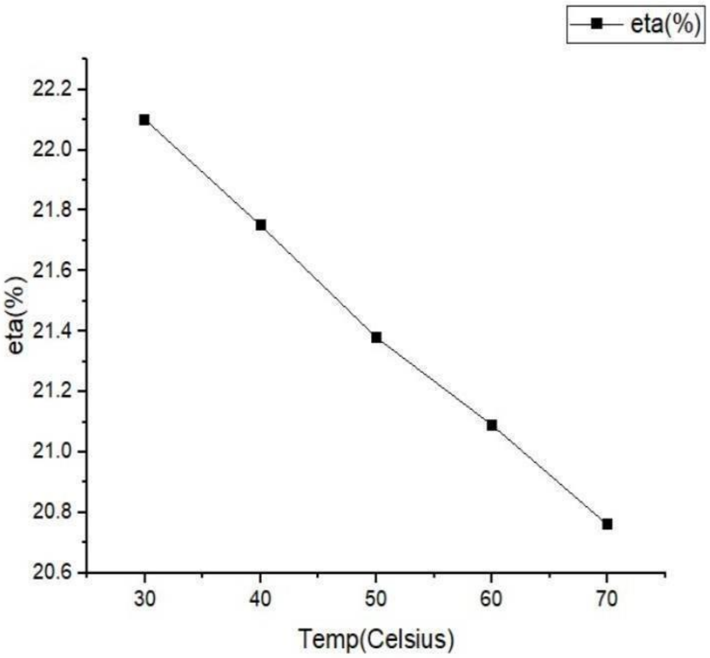

Figure 5.1.10: Effect of Temperature(Celsius) on eta(%)

# CONCLUSION

Simulated the solar cell with PEDOT: PSS as HTL material and concluded the PEDOT: PSS as the better material for HTL with thickness of 50nm. Simulated the solar cell with different thickness of Active Layer CH4N2SnI3 and concluded the thickness as 500nm.Simulated the solar cell with C60 as the ETL material and concluded the thickness of 50nm and the best material is C60nanorod with FaSnI3 as an active layer. The optimized structure is Glass/FTO/PEDOT: PSS/CH4N2SnI3/C60/BCP/Ag with the highest efficiency of 23.

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