SOLAR CELLS AND MODELING OF PEROVSKITE(LEAD-FREE) SOLAR CELLS USING SCAPS 1D SOFTWARE

A DISSERTATION REPORT

SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
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DECLARATION

I **Leeladhar Saini (2K22/MSCPHY/24)** hereby certify that the work which is presented in the Major Project-II entitled ***"Solar Cells And Modelling of Perovskite (Lead-Free) Solar Cells Using SCAPS 1D Software"*** in fulfillment of the requirement for the award of the **Degree of Master of Science in Physics** and submitted to the Department of Applied Physics, Delhi Technological University, Delhi is an authentic record of my own work, carried out during a period from July 2023 to June 2024, under the supervision of **Dr. Sarita Baghel**
The matter presented in the thesis has not been submitted by me for the award of any other degree of this or any other Institute/University.

Leeladhar Saini
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SUPERVISOR CERTIFICATE

To the best of my knowledge, the above work has not been submitted in part or full for any Degree or Diploma to this University or elsewhere. I, further certify that the publication and indexing information given by the students is correct.

Place: Delhi
Date: 07/06/2024

Signature of Supervisor
(Dr. Sarita Baghel)

ABSTRACT

Researchers have become interested in double perovskite solar cells due to the high cost of silicon(Si) based solar cells and the toxic nature of lead (Pb) in lead (Pb) based solar cells. We have simulated with the lead (Pb) free Rb_2SnI_6 with the help of SCAPS-1D software. In this study, we use various combinations of different ETL (Electron transport layer) and HTL (Hole transport layer) with absorber layer Rb_2SnI_6. In This SCAPS study, we changed some parameters like electron affinity, thickness, temperature, and defect density and then studied the open circuit voltage(V_{OC}, in volts), Fill factor(FF%), J_{SC} (mA/cm^2), and PCE(%). We got the final perovskite solar cell (FTO/ETL/ Rb_2SnI_6/HTL/Au). Its properties are as follows F.F. (%) 78.01, J_{SC}(mA/cm^2) 33.5705, V_{OC}(V) 0.9354 , and PCE(%) 25.29 at the temp. 300K, thickness 0.800µm, and defect density 10^{13}(cm^{-3}). It's a highly efficient perovskite solar cell.

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LIST OF SYMBOLS

Symbol	Description
J_{SC}	Short Circuit Current
V_{OC}	Open Circuit Voltage
E_g	Bandgap
N_C	Effective density of states in the conduction band
N_V	Effective density of states in the valence band
N_D	Concentration of donor impurities
N_A	Concentration of acceptor impurities

LIST OF ABBREVIATIONS

Abbreviations	Description
PV	Photovoltaic
PSC	Perovskite Solar Cell
FF	Fill Factor
QE	Quantum Efficiency
PCE	Power Conversion Efficiency
HTL	Hole Transport Layer
ETL	Electron Transport Layer
SCAPS-1D	Solar Cell Capacitance Simulator 1D
FTO	Fluorine-doped Tin Oxide

CHAPTER 1

INTRODUCTION

1.1 SOLAR CELL

Photovoltaic (PV) cells, sometimes referred to as solar cells, are gadgets that use the photovoltaic effect to directly convert sunlight into electricity. These solar cells, which are the fundamental building blocks of solar panels, are crucial parts of solar power systems that produce energy.

The operation of solar cells is explained as follows:

Photovoltaic Effect: Semiconductor materials, most often silicon, are used to make solar cells. Photons, or light particles, are absorbed by the semiconductor material in these cells when sunlight touches them.

Electrons in the semiconductor material receive energy from the absorbed photons, which causes them to become excited and break free from their atoms, resulting in the formation of electron-hole pairs.

Electric Field Generation: To generate an electric field across the cell, a certain treatment is applied to the semiconductor material. A current is created when the free electrons are forced to travel in a given direction by this electric field.

Electric current is produced by the solar cell's metal contacts, which intercept the flow of electrons. After that, this current can be converted to energy or saved for later use in batteries.

The materials utilized, cost, and efficiency of solar cells vary. Common solar cell types include the following:

Silicon monocrystalline solar cells: These are high costly but are noted for their great efficiency because they are made of single-crystal silicon.

Silicon solar cells that are polycrystalline (multicrystalline) are constructed from silicon crystals that are made up of several tiny crystals. Compared to monocrystalline cells, they are slightly less efficient but also less expensive.

Photovoltaic material is deposited in thin layers onto a substrate to create thin-film solar cells. Cadmium telluride (CdTe), copper indium gallium selenide (CIGS), and amorphous silicon (a-Si) are examples of thin-film technologies. Compared to crystalline silicon cells, they are often less efficient, although they are less expensive to create.

Technology developments in solar cells keep raising their cost-effectiveness, durability, and efficiency. Consequently, solar energy has gained traction in household, commercial, and utility-scale applications for producing clean power, making it more competitive with conventional fossil fuel-based energy sources.

1.2 WORKING PRINCIPLE OF SOLAR CELL

The process of turning light energy (photons) into electrical energy is known as the photovoltaic effect, and it is the foundation of how a solar cell function. Usually constructed of semiconductor materials, primarily silicon, solar cells include many layers that, when exposed to sunlight, enable the creation and passage of electric current.

This is a thorough explanation of how a solar cell function: Photon Absorption: Photons from sunlight strike the surface of the solar cell and are absorbed by the semiconductor material, which is typically silicon.

Creation of Electron-Hole Pairs: The energy of the absorbed photons is transferred to the semiconductor material's electrons. Some electrons are liberated from their atoms as a result of this energy absorption, forming electron-hole pairs. The valence band has holes, or positively charged spaces, left behind by electrons that have enough energy to transition from the valence band to the conduction band.

Separation of Charges: The material generates an electric field because of the internal structure of the solar cell. Within the semiconductor material, this electric field causes the separated negative (free electrons) and positive (holes) charges to travel in opposing directions.

Current Flow: The separated charges are moved by the electric field inside the solar cell. Whereas the holes travel toward the rear surface of the cell, the liberated electrons travel toward the front surface. These traveling charges are caught by metal contacts on the cell's front and rear surfaces, which produce an electric current.

Production of Electricity: The captured electrons release an electrical current that can be utilized to power gadgets or replenish batteries.

Finishing the Circuit: A solar panel is typically made up of solar cells connected in parallel or series. An array made up of several panels can produce more electricity. The electrical energy produced can be fed into the grid, stored in batteries, or used right away.

1.3 GENERATIONS OF SOLAR CELLS

Over time, solar cells have undergone evolution, and their development can be divided into distinct generations according to breakthroughs in technology, materials utilized, efficiency gains, and manufacturing techniques.

1.3.1 FIRST GENERATION

Crystalline silicon-based solar cells are the main type of first-generation solar cells. These silicon cells, which come in monocrystalline and polycrystalline varieties, rule the market. They have been commercially accessible for several decades and have rather good efficiency rates.

Monocrystalline Silicon Solar Cells: These solar cells have excellent efficiency rates since they are composed of silicon single crystals. They are carved from cylindrical silicon ingots and

have a homogeneous structure. Monocrystalline cells typically have a longer lifespan and use less space. They are frequently utilized in both residential and commercial installations, and their black appearance makes them immediately identifiable.

Multiple crystalline or polycrystalline Silicon Solar Cells: Silicon crystals made up of several tiny crystals are used to create polycrystalline solar cells. To make them, raw silicon is melted and then poured into square molecules. They often have slightly lower efficiency levels than monocrystalline cells but being less expensive to make. Blue-coloured polycrystalline solar cells are widely utilized in a range of solar applications.

1.3.2 SECOND GENERATION

Thin-film solar cells are referred to as second-generation solar cells. Materials such as copper indium gallium selenide (CIGS), amorphous silicon (a-Si), cadmium telluride (CdTe), and other thin-film technologies are used in these cells. They can be made flexible or semi-transparent, and their manufacturing costs are often lower than those of first-generation cells. They usually have lower efficiency than crystalline silicon cells, though.

Photovoltaic materials are deposited in thin layers onto a substrate to create thin-film solar cells. There are various varieties in this category:

Silicon amorphous (a-Si) Solar Cells: Non-crystalline silicon is used to make these cells. Although they are adaptable and have a wide range of uses, they typically perform less efficiently than crystalline silicon cells.

Solar Cells Made of Cadmium Telluride (CdTe): Cadmium and tellurium are combined to form a semiconductor used in CdTe cells. They have a reputation for being reasonably priced and having excellent efficiency rates. Nonetheless, there have been questions expressed over cadmium's toxicity.

Copper, indium, gallium, and selenium are the constituent elements of a thin layer of semiconductor material used to create copper, indium gallium, and selenium (CIGS) solar cells. They can be adaptable and have good efficiency, which makes them appropriate for a range of uses.

1.3.3 THIRD GENERATION

Third-generation solar cells aim to further boost efficiency, lower costs, and improve performance by utilizing a variety of cutting-edge technologies and unique materials to solve the shortcomings of preceding generations. Among the technologies categorized as third generation are:

Perovskite Solar Cells: Owing to their high efficiency potential, low production costs, and simplicity in fabrication, perovskite solar cells have showed significant promise. To increase stability and longevity, research and development are still being done on them.

Organic Photovoltaics (OPVs): These solar panels make use of organic ingredients that can be converted into lightweight, thin, flexible cells. They can be produced at a low cost and used in a variety of creative ways, such building-integrated photovoltaics.

Dye-Sensitized Solar Cells (DSSCs): DSSCs produce electricity by absorbing light and utilizing dyes. They've demonstrated promise for use in low-light environments and are reasonably simple to produce.

CHAPTER 2

PEROVSKITE SOLAR CELL

2.1 INTRODUCTION

Perovskite solar cells are a kind of solar cell that uses materials with a perovskite structure to produce electricity when exposed to sunlight. Since the materials utilized in these solar cells have a similar crystal structure to the mineral perovskite, these materials bear the same name.

2.2 PEROVSKITE STRUCTURE

Compounds utilized in perovskite solar cells are among the materials that have a certain crystal structure, which is referred to as "perovskite" in this context. A particular cubic or tetragonal crystal lattice defines the unique arrangement of the perovskite crystal structure.

- A perovskite compound's general chemical formula is ABX3, where A is a bigger cationic atom or ion that is usually found in the unit cell's centre
- B is a smaller cationic atom or ion that is usually found in the unit cell's corners.
- The anionic group that connects the A and B ions is called X. It is typically a halide ion, such as iodide, bromide, or chloride.
- The bigger A cations occupy the center of the cubic unit cell, with the smaller B cations surrounding them at the corners and connecting them via the X anions, forming a three-dimensional framework that represents the perovskite crystal structure.
- Methylammonium lead iodide (MAPbI3) or its derivatives are an organic-inorganic hybrid that are the most widely utilized perovskite material in perovskite solar cells. The MAPbI3 chemical is composed of methylammonium (MA+) as the A-site cation, lead (Pb2+) as the B-site cation, and iodide (I-) as the anionic group. It has a perovskite crystal structure.

- The way these ions are arranged inside the perovskite structure is essential to the material's photovoltaic capabilities. The key to the perovskite structure's use in solar cells is its capacity to transfer electrical charges, separate charge carriers, and efficiently absorb sunlight.

2.3 BASIC STRUCTURE OF PEROVSKITE SOLAR CELL

A perovskite solar cell's fundamental structure usually consists of many layers that cooperate to transform sunlight into electrical energy. Although there are variances, the fundamental framework consists of the following essential elements:

2.3.1 Substrate

The substrate acts as the solar cell's overall support system and foundation. Glass and flexible materials like plastic or metal foils are frequently utilized substrates that offer structural support and a foundation for higher layers.

2.3.2 Transparent Conductive Oxide Layer(TCO)

This layer is put onto the substrate and is commonly composed of materials such as indium tin oxide (ITO) or fluorine-doped tin oxide (FTO). It functions as a transparent electrode, permitting the extraction of generated electrical current while permitting light to reach the active layers.

2.3.3 Hole Transport Layer (HTL)

It allows the passage of positively charged "holes" created by layers that absorb sunlight. The HTL can be composed of either biological or inorganic materials. Conductive polymers, the well-liked organic substance Spiro-OMeTAD, and transition metal oxides are examples of HTL materials that are frequently utilized.

2.3.4 Perovskite Absorber Layer

Methylammonium lead iodide (MAPbI3) or other such compounds make up the perovskite substance that forms the core of the perovskite solar cell. The photovoltaic process is started by the perovskite layer's absorption of sunlight, which creates electron-hole pairs.

2.3.5 Electron Transport Layer (ETL)

Negatively charged electrons produced by the absorbed sunlight are moved more easily by the Electron Transport Layer (ETL). In order to transfer electrons, materials like titanium dioxide (TiO2), zinc oxide (ZnO), or other metal oxides are frequently utilized in this layer.

2.3.6 Back Contact or Electrode

By offering an electrical contact for the extraction of electrons produced during the photovoltaic process, the back electrode layer completes the structure of the solar cell. Materials like aluminium, silver, and gold are frequently used.

Through the transparent conductive oxide layer, sunlight enters the cell and is absorbed by the perovskite layer. This absorption produces pairs of electrons and holes. Whereas holes flow toward the hole transport layer, electrons flow toward the electron transport layer. The front and back contacts of the corresponding electrodes gather the separated charges, producing an electrical current that can be utilized to generate power.

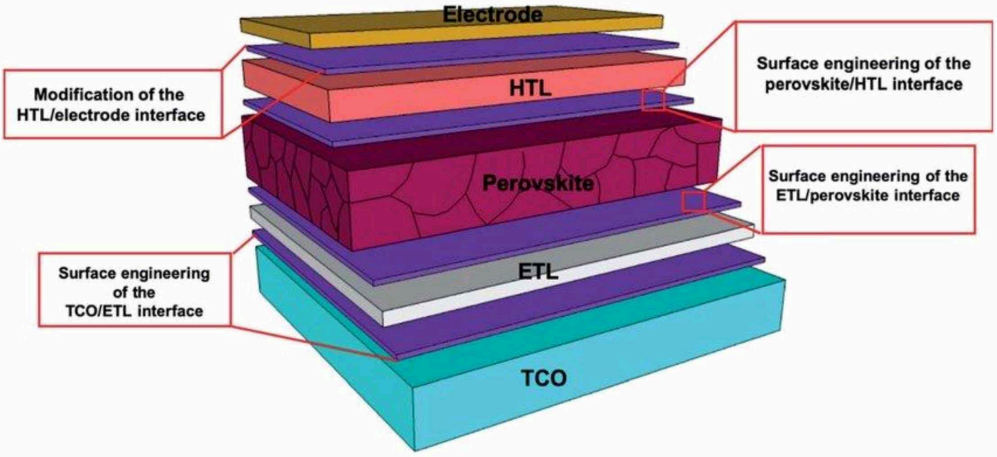

Fig 2.1 Basic structure of Perovskite solar cell.

2.4 ADVANTAGES

The following are some salient features of perovskite solar cells:

- Materials Used: Perovskites are a family of materials that have a particular crystal structure that are used in perovskite solar cells. Methylammonium lead halide, often known as methylammonium lead iodide, is the most widely used perovskite material for solar cells.
- High Efficiency: The remarkable efficiency of perovskite solar cells in converting sunlight into electricity has drawn attention to them. They have quickly attained excellent power conversion efficiencies; in lab settings, they have even surpassed certain conventional silicon-based solar cells.
- Low Production Costs: The synthesis of perovskite materials can be achieved at a comparatively low cost utilizing readily available ingredients. Due to their potential for economical production, perovskite solar cells may prove to be a more cost-effective substitute for conventional silicon-based solar cells.
- Versatility: Solution-based techniques can be used to manufacture perovskite solar cells into thin films, providing versatility in terms of design and use. Because of their

adaptability, they can be used in a wide range of contexts, such as building materials, portable electronics, and other creative applications.

2.5 CHALLANGES OF PEROVSKITE SOLAR CELL

The issues surrounding perovskite solar cells—namely, how to improve their stability, scalability for mass production, and commercial viability—remain the focus of research and development activities. Perovskite solar cells are a promising option for the upcoming generation of solar photovoltaics, with the potential to contribute to the evolution of clean and sustainable energy technologies due to their high efficiency and rapid progress.

CHAPTER 3

SIMULATION AND METHODOLOGY

3.1 SCAPS 1D (Solar Cell Capacitance Simulator)

A software program called SCAPS (Solar Cell Capacitance Simulator) is used to model and simulate the operation of different kinds of solar cells. The goal of SCAPS, which was created at the University of Gent in Belgium, is to evaluate and forecast solar cell properties depending on various materials, structures, and configurations.

Key characteristics of SCAPS version 3.3.10 are as follows:

- A solar cell's structure can have up to seven semiconductor layers.
- Various recombination processes are permitted, including Auger, direct, and SRH type.
- A defect level can have specifications for optical characteristics, energy distribution, charge type, and many other disciplines.
- Metal contacts that are allocated a work function or a flat band option.
- The application has predefined solar spectra for illumination, such as AM0, AM1.5D, AM1.5G, monochromatic, white, etc.
- There are options for front or rear device illumination.
- A variety of computations, including QE curves, I-V, C-V, C-f, and energy band diagrams, can be done.
- Calculations in batches are possible, and variations about batch parameters can be displayed.

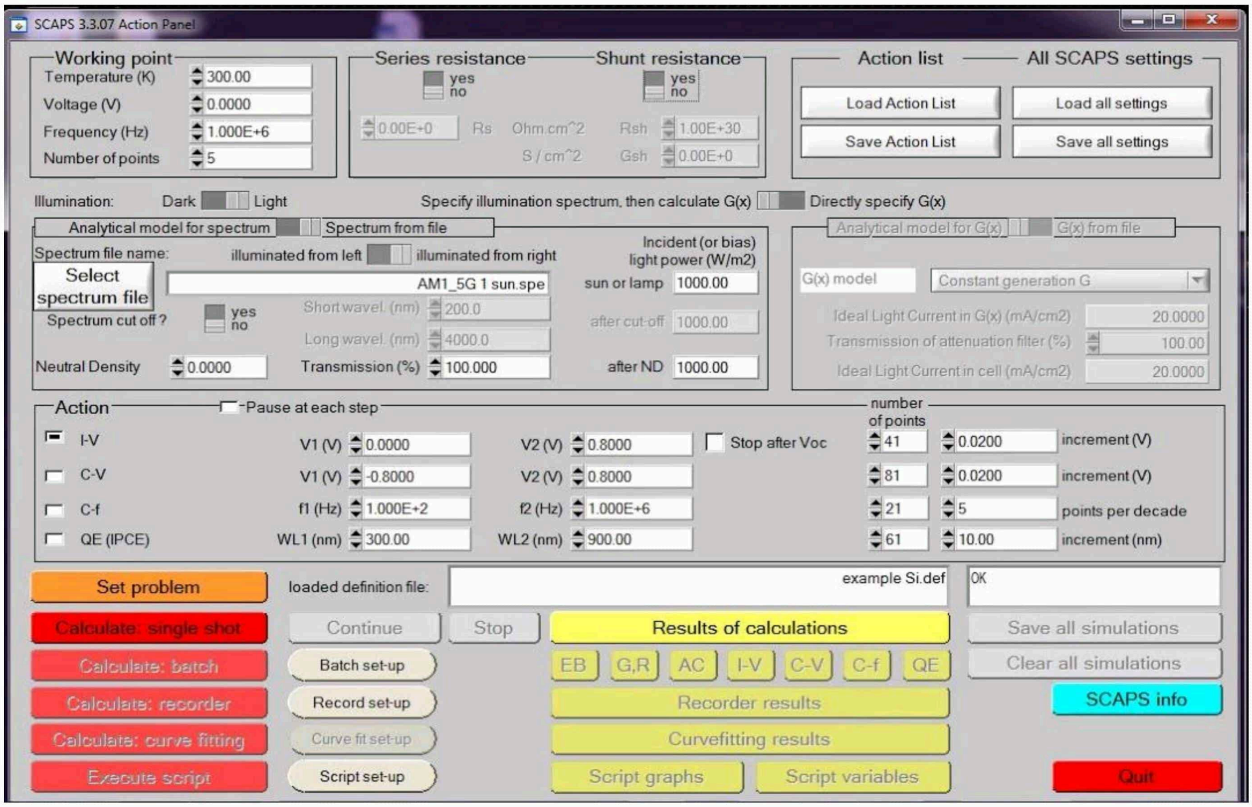

Fig 3.1 SCAPS 1D SIMULATOR

Fig 3.2 Cell structure in SCAPS.

3.2 PEROVSKITE SOLAR CELL DESIGN IN SCAPS-1D

To make a perovskite solar cell, we first have to follow the basic steps.

- First of all we open the SCAPS 1D software screen of our laptop or desktop
- We click on the Set a Problem section
- Now we use different layers here. In this part, we can define our metal connections, layer order, and cell structure.
- Put the numerical values in different layers. Put the properties like bandgap, the thickness of the layer, electron and hole mobility, defect, electron affinity, dielectric permittivity, And the density of states in different layers.
- We modify our software according to the properties of the material such as temperature, light intensity, resistance, voltage, and interface properties so that we can achieve maximum efficiency.
- TO perform the simulations in SCAPS 1D. By doing the simulation we get our results such as efficiency, fill factor, current density, And open circuit voltage. By performing simulations. we get current-voltage characteristics, capacitance-voltage characteristics, And quantum efficiency curve.
- We continue to monitor our results and perform simulations in order to identify the best efficient solar cell. This could mean looking into how the device works, modifying settings, comparing different buildings, or finding relevant figures of merit.

  A simulation model for lead-free Rb_2SnI_6 perovskite solar cells was set up in SCAPS 1D to study the effect of the change of thickness of the absorber layer and ETL on device parameters.

A simulation model for lead-free Rb_2SnI_6 perovskite solar cells was set up in SCAPS to study the effect of the change of thickness of the absorber layer and ETL on device parameters.

3.3 NUMERICAL ANALYSIS OF Rb_2SnI_6

The following are the parts of the solar gadget that are studied

We design a cell (Au/Cu_2O/Rb_2SnI_6/ZnSe/FTO), here Au is back contact, Cu_2O is the hole transport layer, Rb_2SnI_6 is the light absorber layer, and ZnSe is an electron transport layer. The creation of the aforementioned cell structure is shown in Fig. 3.1. The special properties of Rb2SnI6, and FTO are listed in Table 3.1 come from a variety of theoretical and experimental studies that have been made available to the general public [8,26]. The researchers discovered that the experimental band gap of Rb2SnI6 is 1.32 eV[3,9]. We used the SCAPS-1D program to improve the photovoltaic (PV) performance of the PSC [19,5]. This theoretical and computational work suggests that Rb2SnI6 can provide excellent and reliable PV performance in photovoltaic applications as a suitable lead halide perovskite substitute. The band gap of FTO is 3.5eV [7,1] and the work function of Au is 5.1eV[10].

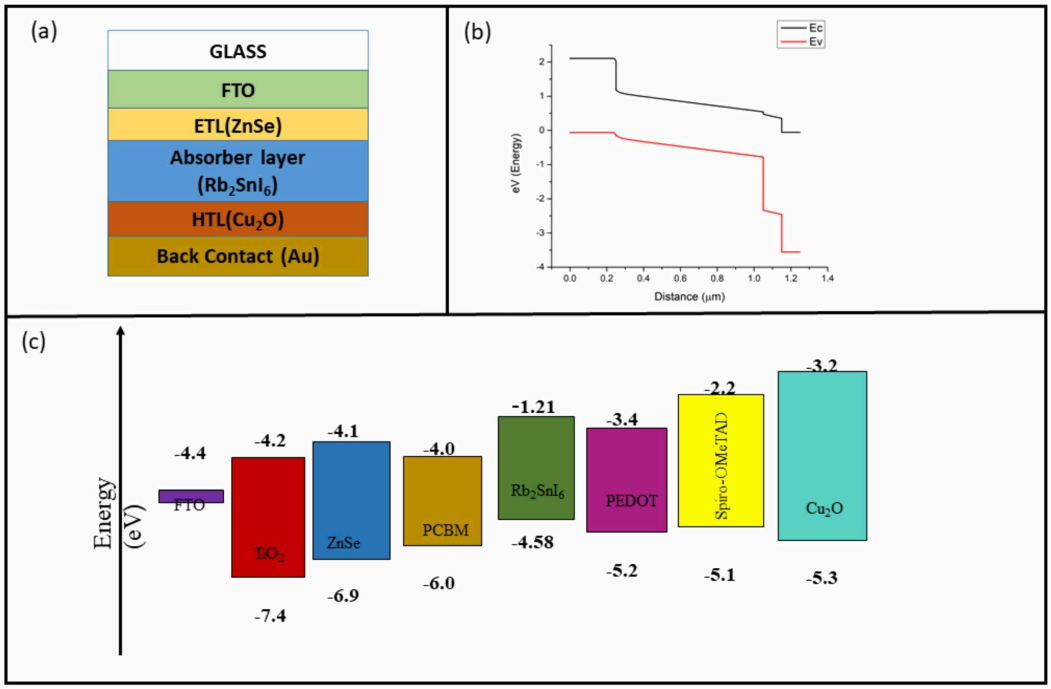

Fig 3.3 (a) Perovskite solar cell (b) Energy band diagram of different layers with connections (c) Energy band diagram of different solar cell materials without connections

Table 3.1 Numeric values for perovskite layer and transparent conductive oxide layer

Parameters	*Rb_2SnI_6*	*FTO*
Thickness(m)	800	100
Band gap(eV)	1.32	3.5
Electron Affinity(eV)	4.023	4.5
ε/ε0(Dielectric permittivity)	16.6	9
CB Density of states(cm^{-3})	4.580×10^{19}	2.2×10^{18}
VB density of states(cm^{-3})	1.80×10^{20}	1×10^{19}
Electron mobility($cm^2V^{-1}S^{-1}$)	38.6	2×10^{3}
Hole mobility($cm^2V^{-1}S^{-1}$)	14.9	2×10^{3}
Donor Density(cm^{-3})	7.15×10^{9}	2×10^{19}
Acceptor Density(cm^{-3})	7.15×10^{9}	0
Defect Density(cm^{-3})	1×10^{13}	1×10^{15}
Reference	[4,5]	[7,1]

Table 3.2 Different Electron Transport Layers (ETL)

Parameters	*ZnSe*	*IGZO*	*TiO_2*
Thickness(nm)	100	100	100
Band gap(eV)	2.81	3.050	3.2
Electron Affinity(eV)	4.09	4.160	4
ε/ε0(Dielectric permittivity)	8.6	10	9
CB Density of states(cm^{-3})	2.2×10^{18}	5×10^{18}	2×10^{18}
VB density of states(cm^{-3})	1.8×10^{18}	5×10^{18}	1.8×10^{19}
Electron mobility($cm^2V^{-1}S^{-1}$)	400	1.5	20
Hole mobility($cm^2V^{-1}S^{-1}$)	110	0.1	10
Donor Density(cm^{-3})	1×10^{15}	1×10^{17}	9×10^{16}
Acceptor Density(cm^{-3})	0	0	0
Defect Density(cm^{-3})	1×10^{15}	1×10^{15}	1×10^{15}
Reference	[1,8]	[9,1,11]	[1,10]

3.3 Table Different Hole Transport Layers(HTL)

Parameters	*Cu_2O*	*Spiro-OMeTAD*	*PEDOT: PSS*	*CBTS*
Thickness(nm)	250	200	200	200
Band gap(eV)	2.17	3	1.6	1.9
Electron Affinity(eV)	3.2	2.2	3.4	3.6
ε/ε0(Dielectric permittivity)	7.11	3	3	5.4
CB Density of states(cm^{-3})	2.02×10^{17}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}
VB density of states(cm^{-3})	1.1×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Electron mobility($cm^2V^{-1}S^{-1}$)	200	2.1×10^{-3}	4.5×10^{-2}	30
Hole mobility($cm^2V^{-1}S^{-1}$)	80	2.16×10^{-3}	4.5×10^{-2}	10
Donor Density(cm^{-3})	0	0	0	0
Acceptor Density(cm^{-3})	1×10^{18}	1×10^{18}	1×10^{18}	1×10^{18}
Defect Density(cm^{-3})	1×10^{14}	1×10^{15}	1×10^{15}	1×10^{15}
Reference	[1,23,27]	[29,28,30]	[22,23]	[23,2,1]

CHAPTER4

RESULT AND DISCUSSION

4.1 Rb_2SnI_6

As previously mentioned, we used several ETLs and HTLs to model several unique Double Perovskite solar cells. The simulation data was then captured.

Table 4.1 Different cell arrangements and the results of their simulations

Cell structure (*FTO/ETL/ Rb_2SnI_6/HTL/Au*)	*V_{OC}(V)*	*J_{SC}(mA/cm^2)*	*FF(%)*	*PCE(%)*
Au/Cu_2O/Rb_2SnI_6/TiO_2/FTO	0.9354	33.8705	78.01	24.74
Au/Cu_2O/Rb_2SnI_6/ZnSe/FTO	0.9350	33.8967	79.79	25.29
Au/Cu_2O/Rb_2SnI_6/IGZOFTO	1.585	33.6485	46.88	25.01
Au/Spiro-OMeTAD/Rb_2SnI_6/ZnSe/FTO	0.9346	33.8678	77.65	23.78
Au/ Spiro-OMeTAD /Rb_2SnI_6/ TiO_2//FTO	0.9346	33.8678	77.65	23.64
Au/ Spiro-OMeTAD /Rb_2SnI_6/ZnSe/FTO	0.9342	33.8941	79.43	25.15
Au/PEDOT:PSS/Rb_2SnI_6/IGZO/FTO	1.5890	33.6702	46.90	24.95
Au/PEDOT:PSS/Rb_2SnI_6/TiO_2/FTO	0.9358	33.8946	77.89	24.70
Au/PEDOT:PSS/Rb_2SnI_6/ZnSe/FTO	0.9352	33.9966	79.66	25.28
Au/CBTS/Rb_2SnI_6/IGZOFTO	15872	33.6530	46.83	25.02
Au/CBTS/Rb_2SnI_6/ZnSe/FTO	0.9351	33.9011	79.79	25.29
Au/ CBTS/Rb_2SnI_6/ TiO_2//FTO	0.9355	33.8749	78.02	24.72
Au/CuO/Rb_2SnI_6/TiO_2/FTO	0.8208	33.9447	77.35	21.55

Au/MASnBr$_3$/Rb$_2$SnI$_6$/TiO$_2$/FTO	0.9356	33.8696	77.94	24.70
Au/ MASnBr$_3$/Rb$_2$SnI$_6$/IGZO/FTO	1.5773	33.6477	47.15	25.02
Au/ MASnBr$_3$/Rb$_2$SnI$_6$/ZnSe/FTO	0.9352	33.8946	79.72	25.27

the values of Voc (volt), Jsc (mA/cm^2), FF (%), and PCE (%) that correlated with the indicated device structure (FTO/ETL/ Rb_2SnI_6/HTL/Au) were obtained from the pertinent simulations. Furthermore, the information required for different graphs and analyses was noted. We found that FTO/ZnSe/ Rb_2SnI_6/Cu_2O/Au is our ideal combination after conducting this experiment.

4.2 Variation in Temperature

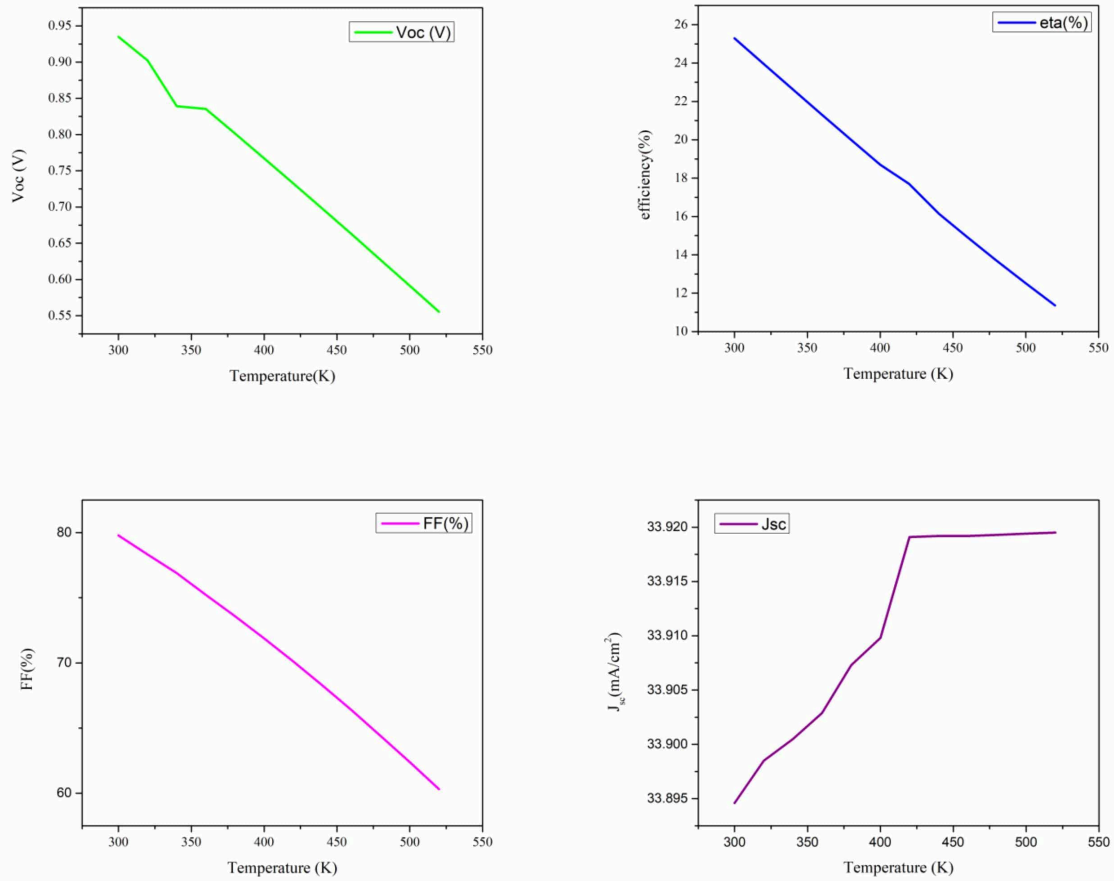

Fig 4.1 effect of temperature

The temperature at which a solar cell operates has a significant impact on its performance. When the simulation was run with temperatures ranging from 300 K to 520 K with a continuous light source and temperature was found to be 300 K.

Increased temperatures have the potential to impact material properties such as band gap energies, electron and hole mobility, and carrier concentration, which can ultimately result in a reduction of cell efficiency [23,34]. The effects of temperature on J_{SC}, V_{OC}, F.F., and PCE are depicted in Figure 4.1. The figure illustrates how a rise in temperature causes a drop in volatile organic compounds. The operating temperature has no effect on current density because of the inevitable voltage drop. It is shown that the F.F. initially rises with

temperature before suddenly falling. When comparing the perovskite to the

The layer is 0.8 µm thick, the temperature is 300 K, and the PCE and F.F. are at their highest levels.

This illustrates the characteristics of the cell with a 1.35 band gap and a 0.8 µm absorber, such as V_{OC}, F.F., J_{SC}, and PCE, at temperatures between 300 K and 520 K [24,27]

4.3 Variation in Thickness

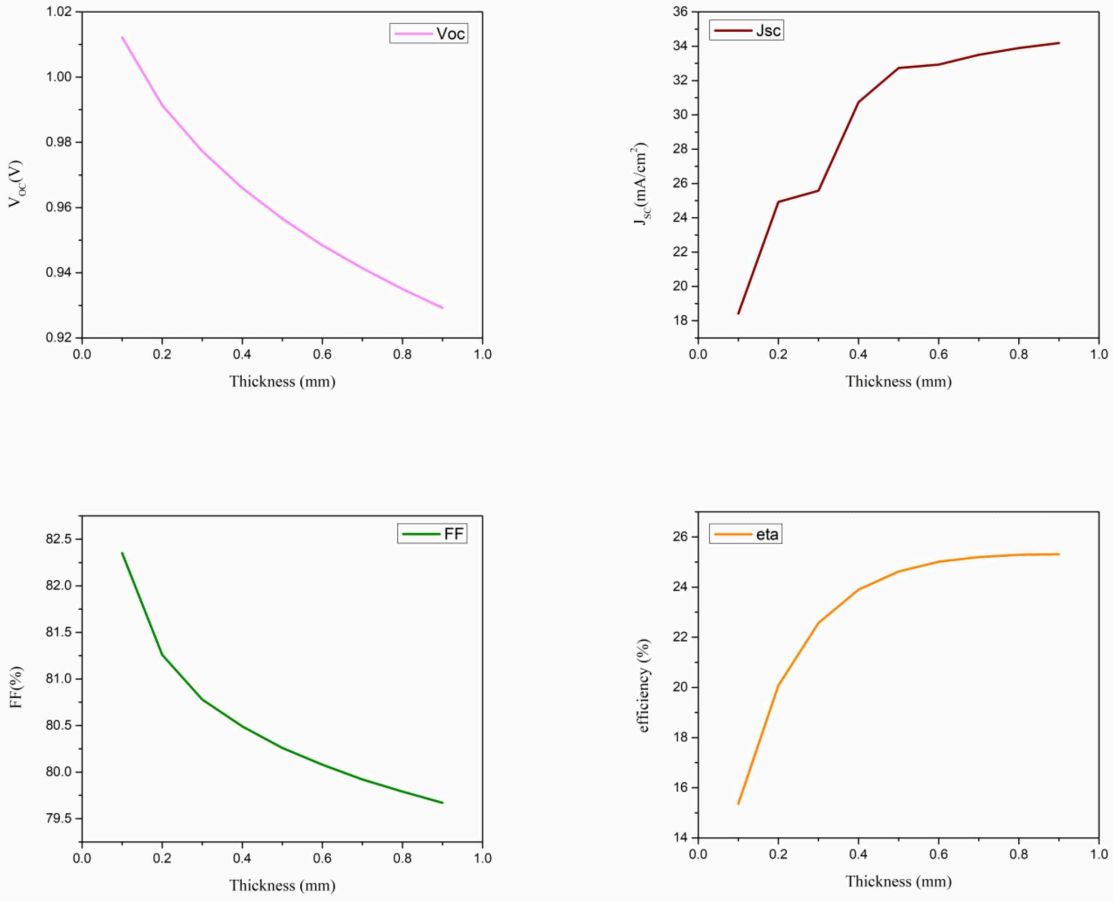

Fig. 4.2 Effect of variation in Thickness

The "thickness of the absorber layer" of a perovskite solar cell greatly affects its performance. Changing the thickness of the absorber layer can have the following effect

- The size of the absorber layer directly affects its ability to absorb light[16]. The number of electron-hole pairs produced may rise with the size of the absorber layer if

it is able to absorb more light[15]. At the front and rear interfaces,

Due to light absorption and reflection, absorber layers that are too thick may potentially cause significant losses.

- The distance that the produced charge carriers must travel to reach the ETL and HTL is determined by the breadth of the absorber layer. Overly thick absorber layers may make it more likely for charge carriers to recombine before being collected. However, there's a chance that an incredibly thin absorber layer won't be able to generate and capture enough charge carriers.
- It is the highest current output of a solar cell, and it is directly influenced by the perovskite layer's width. Increases in absorber layer thickness often cause the JSC to rise to a certain degree before plateauing or

  decreases due to a rise in recombination losses.
- The thickness of the absorber layer can have an impact on the maximum voltage, or V_{OC}, that a solar cell can generate. Sometimes a higher density of states or more trap-assisted recombination results in thickening of the perovskite layer[13].

  reduces the amount of V_{OC}.
- The unit of measurement for a cell's capacity to convert light into electrical current is F.F. A greater F.F., which denotes successful charge carrier collection and fewer losses, may be obtained with appropriate thickness.
- The overall performance of a PSC is significantly influenced by the thickness of the absorber layer[35]. The processes of light absorption, charge carrier production, collection, and recombination losses can all be balanced with the right thickness. Reduced PCE could

  if the thickness is not maintained uniformly[17]

- Optimising the thickness of the absorber layer is necessary for a photovoltaic solar cell (PSC) to attain the optimal equilibrium among light absorption, charge carrier production, and collection. For different device configurations and material compositions, there may be different optimum thickness ranges.[36]
  Research using computational and experimental methods is often used to establish the ideal thickness of the absorber layer for a given PSC design[21].

4.4 Variation in defect density

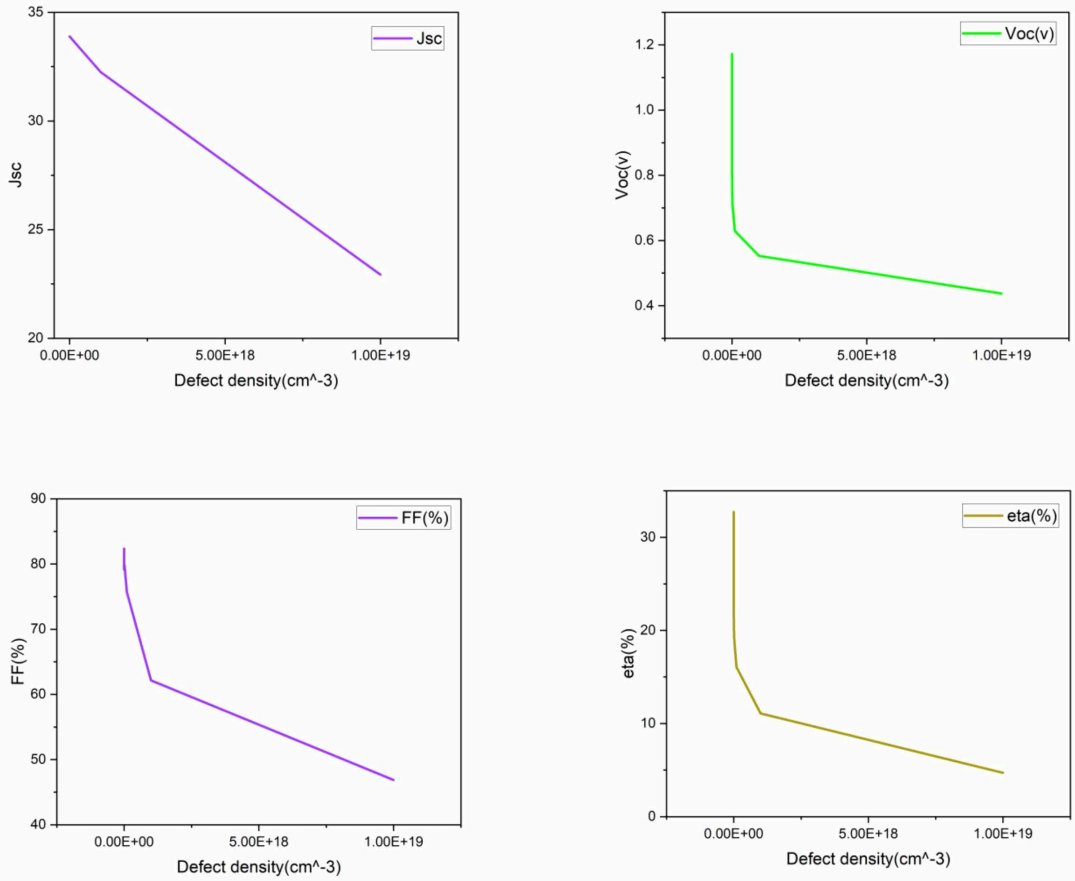

Fig 4.3 Variation in defect density

To investigate the impact of a change in defect density in the Rb_2SnI_6-layer on the PCE and other parameters of the Rb_2SnI_6 solar cell, batch calculations were performed in SCAPS-1D. Steps of 101 were used to vary the Defect Density, Nt.

at a consistent 800 nm thickness. When we maintained the same values for all other ETL, HTL, FTO, and absorber layer parameters as shown in Table 3.1, we saw a drop in DPSC efficiency as Nt increased. Efficiency varied very little below Defect Density Nt = 10^{11} cm-3. When efficiency reaches 32.74%, defect density exceeds this threshold.

The solar cell's efficiency drops dramatically, reaching 22.25% at 1.3×10^{13} and 4.70% at 1.3×10^{18}. One important factor that affects the device's efficiency is the value of N_t in the active layer[12]. Pinholes are created when there is a high concentration of flaws, which

increases recombination[31]. Additionally, it decreases stability, speeds up the deterioration of coatings, and generally deteriorates device performance[31,18].

CHAPTER 5

CONCLUSION

Tuning the absorber layer thickness, temperature, band gap, and electron affinity results in a higher PCE. It seems that the PCE climbs and eventually lowers to a specific amount as absorber thickness increases. The layer's carrier concentration is absorbing more photons, which results in the production of more electron-hole pairs and a rise in the short-circuit current density of the device. Additionally, PCE is evaluated at different temperatures, and it is shown that as the band gap widens, the efficiency decreases. Finding the PCE for changing electron affinity shows that when electron affinity rises or falls and with different temperatures PCE shows efficiency will decreases and the efficiency of solar cells it depends on different parameters.

After examining the effects of different ETLs and HTLs on PSCs, we found that the most effective combination was ZnSe for the ETL and Cu_2O for the HTL. We have examined the correlation between several parameters, such as Nt, operating temperature, and absorber layer thickness. use the SCAPS-1D simulator program to modify the device's characteristics. The device structure Au/Cu_2O/Rb_2SnI_6 /ZnSe /FTO for 800 nm thickness has attained the highest PCE of 25.29%, based on the simulation results. The ideal Nt value and temperature for the PSC are 10^{13} units and 300 K, respectively.

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