Investigating the efficiency and optimizing of Germanium-based Perovskite Solar Cell using SCAPS 1D

A DISSERTATION

SUBMITTED IN FULFILLMENT OF THE REQUIREMENTS FOR THE

AWARD OF THE DEGREE

OF

MASTER OF SCIENCE

IN

PHYSICS

Submitted by:

Vanshika (2K21/MSCPHY/50)

&

Anushansha Yadav (2K21/MSCPHY/60)

Under the Supervision of

Dr. Sarita Baghel

DEPARTMENT OF APPLIED PHYSICS

DELHI TECHNOLOGICAL UNIVERSITY

(Formerly Delhi College of Engineering)

Bawana Road, Delhi – 110042

MAY, 2023

2

SUPERVISOR CERTIFICATE

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

Dr. Sarita Baghel

SUPERVISOR

Place:Delhi

Date: 31-05-2023

ACKNOWLEDGEMENT
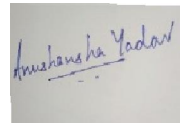
We would like to express our gratitude to our supervisor, Dr. Sarita Baghel for her invaluable feedback and patience. This journey would not have reached completion without her generous support and guidance.

We are also grateful to our batchmates for their moral support and feedback sessions. We would also like to thank the research assistants and librarians of the university for inspiring us.

Lastly, we would like to thank our families for keeping our spirits high and maintaining a strong belief for us.

VANSHIKA

ANUSHANSHA YADAV

ABSTRACT

Germanium-based perovskite solar cells (PSCs) are a substitute for conventional lead-based perovskite solar cells (PSCs) without sacrificing the environment. In this work, simulation has been carried out with the $CsGeBr_3$ perovskite solar Cell on SCAPS-1D and the impact of several factors such as the thickness of the absorber layer, operating temperature and defect density is analyzed. The device has achieved maximum power conversion efficiency (PCE) of 11.35 % with an absorber layer thickness of 600 nm at 305 K. The photovoltaic parameters show that the solar devices are stable at 305 K. This indicates that $CsGeBr_3$ PSC is a promising device for future photovoltaic applications and for designing highly efficient lead-free PSC.

CONTENTS

Title Page	
Declaration	**i**
Supervisor's Certificate	**ii**
Plagiarism Report	**iii**
Acknowledgement	**iv**
Abstract	**v**
Contents	**vi**
List of Figures	**vii**
List of Tables	**viii**
List of Symbols and Abbreviations	**ix**
Chapter 1 INTRODUCTION 1.1 Generations of Solar Cell	

Chapter 2   PEROVSKITE SOLAR CELL
      2.1 History
      2.2 Basic Structure
            2.2.1 Mesoporous Structure
            2.2.2 Plane Heterostructure
            2.2.3 Perovskite Light Absorbing Layer	

LIST OF FIGURES

Chapter 3

Chapter 4

LIST OF TABLES

Chapter 3

Table 3.1: Parameters for material used in this simulation.

Chapter 4

Table 4.1 Performance of solar cells employing different combinations of various elements as ETL and HTL.

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	F.F.
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

Solar cells are technology that converts sunlight into energy. They are a crucial part of solar panels or modules, which are used to capture solar energy for a variety of uses, including the production of electricity. The photovoltaic effect is the basis for how solar cells work. An electric current is produced when sunlight shines on a solar cell's surface by igniting electrons in the semiconductor material of the cell. It is possible to harness this current and use it as a source of electric power. The most popular solar cell component is crystalline silicon (c-Si), which is widely available, efficient, and long-lasting. Crystalline silicon solar cells come in two major varieties:

1. Monocrystalline silicon (mono-Si) cells: The single crystal structures are used to create these cells and have a uniform appearance with rounded edges. They offer high efficiency but are costly to manufacture[1].

2. Polycrystalline silicon (poly-Si) cells: These cells exhibit a fragmented appearance and possess a bluish hue due to the utilization of multiple silicon crystals in their production. They are less expensive to produce but have slightly lower efficiency compared to mono-Si cells[2].

In addition to crystalline silicon, there are also thin-film solar cells that use different semiconductor materials. These include :

1. Amorphous silicon (a-Si) cells: These cells may be deposited on flexible substrates and employ non-crystalline silicon, making them appropriate for flexible solar panels.

2. Cadmium telluride (CdTe) cells: CdTe cells employ a semiconductor material composed of a thin film of cadmium telluride. They are known for their cost-effectiveness and have been used in utility-scale solar power plants.

3. Copper Indium Gallium Selenide (CIGS) cells: These cells use a thin layer of compound like Cu, In, Ga and Se as the semiconductor material. They offer good efficiency and flexibility.

Solar cells have become increasingly efficient and affordable over time, making photovoltaic energy a viable and sustainable source of electricity.

1.1 GENERATIONS OF SOLAR CELL

Solar cells have undergone several generations of development over the years. Each generation represents a significant advancement in terms of materials, efficiency, and manufacturing techniques. Here is an overview of the various generations of solar cells:

1. First Generation (1G): 1G solar cells are predominantly based on crystalline silicon technology, which is the most common used material in solar cells today. These cells, which feature a single p-n junction, dominate the global photovoltaic market and constitute the majority of solar cell installations worldwide.
2. Second Generation (2G): Thin-film innovations including amorphous silicon (a-Si), CdTe, and CIGS are used in 2G solar cells. These cells are constructed using thinner semiconductor material layers, which lowers the cost of the raw ingredients and enables the production of flexible and lightweight solar panels.
3. Third Generation (3G): This generation encompasses a diverse range of emerging technologies aimed at further improving efficiency and reducing costs. These include:
   - Organic solar cells: These cells use organic semiconducting materials, often polymers, to generate electricity. Though they presently have lesser efficiency than silicon-based cells, they do have the potential for low-cost, mass manufacturing.
   - Dye-sensitized solar cells (DSSC): In DSSCs, a layer of dye molecules absorbs photons, which then transmits the energy to a semiconductor material to generate electricity. They are known for their aesthetic appeal and can work well under low-light conditions but have moderate efficiencies.

- Perovskite solar cells (PSC): They are a promising and rapidly progressing technology. They utilize perovskite materials as the photon-absorbing layer, offering high efficiency and low-cost manufacturing. However, stability and longevity remain areas of active research.

- Quantum dot solar cells: QDSCs employ semiconductor nanoparticles (quantum dots) that exhibit quantum confinement effects to enhance their light-absorption properties. They have the potential for high efficiencies and tunable bandgaps[3].

4. Fourth Generation (4G): Research on fourth-generation solar cells is ongoing . They aim to overcome the limitations of previous generations by exploring advanced concepts such as multi-junction solar cells, tandem structures, and novel materials. These technologies target even higher efficiencies, improved durability, and reduced costs.

CHAPTER 2

PEROVSKITE SOLAR CELL

2.1 HISTORY

The history of perovskite solar cells (PSCs) is relatively recent, with significant progress and breakthroughs achieved in the past decade. Here is a quick rundown of the significant turning points in the evolution of PSCs:

2009: Tsutomu Miyasaka and his colleagues in Japan released the first study on PSCs. They used $CH_3NH_3PbI_3$, a perovskite material, as the photon-absorbing layer and got a PCE of about 3.8%.

2012: Researchers at the University of Oxford, led by Henry Snaith, made a breakthrough by adding a solid-state hole conductor in place of the cell's liquid electrolyte, which increased stability. This development helped to boost the performance of PSCs to about 10%.

2013: The efficiency of PSCs rapidly increased to over 15% with various optimizations in device architecture and materials. The use of different compositions and engineering approaches allowed for better charge transport and reduced recombination losses.

2014: PSCs achieved a significant milestone with a reported efficiency exceeding 20%. This rapid improvement attracted significant attention from the scientific community and industry, sparking further research and development efforts.

2016: PSCs reached a record efficiency of over 22%. Researchers explored tandem structures, where perovskite cells were combined with other solar cell technologies like silicon or CIGS, to achieve even higher efficiencies.

2018: The stability and durability of PSCs remained a challenge, but progress was made in improving the long-term performance. Encapsulation techniques and engineering strategies were implemented to enhance the stability and protect the perovskite materials from moist, heat, and light-induced degradation.

2020: The efficiency of PSCs has shown consistent improvement over time, with reports of PCE exceeding 25%. Further advancements were made in materials, device architectures, and manufacturing processes, bringing PSCs closer to commercial viability.

2021-2023: Ongoing research focuses on revitalizing the stability, scalability, and commercialization of PSCs. Efforts are directed towards addressing issues related to moisture, thermal stability, the toxic nature of lead-based compositions, and large-scale manufacturing techniques[4].

The field of PSCs remains dynamic, with new discoveries and advancements being made regularly. The rapid progress and potential of PSCs have positioned them as one of the most optimistic emerging technologies in the solar energy industry, delivering solar cells that are exceptionally efficient, cost-effective, and adaptable.

2.2 BASIC STRUCTURE

A perovskite solar cell's fundamental construction generally consists of many layers that work in concert to absorb and transform sunlight into power. Here is a concise breakdown of the essential elements:

1. Substrate: The bottom layer of the PSC is the substrate, which provides mechanical support and stability to the cell. It is usually made of glass or a flexible material like plastic.
2. Transparent Conductive Layer: A transpicuous conductive layer, often composed of Indium Tin Oxide (ITO) or a transparent conducting polymer, is on the top of the substrate. This layer functions as an electrode for gathering the produced electric current while allowing light to pass through.
3. Electron Transport Layer (ETL): The ETL is a layer that enhances the transfer of electrons in the cell. Commonly used materials for the ETL in PSCs include titanium dioxide (TiO_2) or other metal oxides. The ETL helps remove electrons from the absorbing layer and allows them to flow toward the electrode.

4. Perovskite Layer: The perovskite layer, which absorbs sunlight and produces electrical charges, is the vital component of the solar cell. The substance used to make it is often a hybrid organic-inorganic metal halide perovskite known as $CH_3NH_3PbI_3$. The perovskite layer has excellent light-absorbing properties and converts photons into excited electrons and holes [5, 6].

5. Hole Transport Layer (HTL): This layer assists in moving the positively charged holes produced in the absorber layer. Commonly used materials for the HTL include organic small molecules or polymers. The HTL helps collect the holes and guide them towards the electrode.

6. Contact/Counter Electrode: Above HTL, there exists a contact electrode which is commonly composed of metals such as gold, silver, or carbon-based materials. This electrode collects the holes produced in the perovskite layer and completes the electric circuit.

It's important to note that the actual structure and specific materials used in PSCs may vary depending on the research or commercial development. Researchers continue to explore different device architectures and materials to optimize performance, stability, and manufacturability of PSCs[5].

2.2.1 MESOPOROUS STRUCTURE

The mesoporous structure is the common approach used in the construction of PSCs. It involves incorporating a mesoporous layer within the device architecture to enhance the outcomes of the solar cell. Here's an overview of the mesoporous structure in PSCs[7]:

1. Substrate: This layer is generally composed of glass or a flexible material provides mechanical support and stability.

2. Transparent Conductive Layer: There is a transparent conductive layer above the substrate, such as ITO or a transparent conducting polymer, which allows light to pass through and acts as the electrode for collecting the generated electric current.

3. Mesoporous Layer: The mesoporous layer is situated between the transparent conductive layer and the perovskite layer. It is typically composed of a porous material, such as mesoporous titanium dioxide (TiO_2) or other metal oxides.

The mesoporous structure provides several benefits to the PSC:

Enhanced Light Absorption: The mesoporous layer provides a large surface area and interconnected pores, increasing the interface for light absorption. This enables more efficient utilization of incoming photons, enhancing the overall photon-harvesting ability of the solar cell.

Electron Transport Pathway: The interconnected network of pores within the mesoporous layer allows for efficient transport of electrons generated in the perovskite layer. The mesoporous material, such as TiO_2, acts as an electron conductor, facilitating the movement of electrons toward the electrode.

Increased Perovskite Layer Surface Area: The mesoporous structure creates a high surface area, which can be advantageous for the accumulation of the absorber layer. The perovskite layer has better coverage and homogeneity due to the porous structure's increased availability of sites for the material's nucleation and growth.

Improved Stability: Perovskite solar cells' stability may also be aided by the mesoporous structure. By preventing direct association between the perovskite material and the electrode, the mesoporous layer can lessen the risk of deterioration brought on by unintended reactions.

It's important to note that while the mesoporous structure has shown promise in improving the efficiency of PSCs, there are alternative device architectures and materials being explored. Ongoing research focuses on optimizing the mesoporous structure, as well as developing non-mesoporous approaches, to further improve thePSCs' performance, stability, and scalability

2.2.2 PLANE HETEROSTRUCTURE

A plane heterostructure is an alternative device architecture used in PSCs to improve their performance and steadiness. In a plane heterostructure PSC, the layers are arranged in a planar or stacked configuration. Here's an overview of the plane heterostructure in PSCs:

1. Substrate: The bottom layer of the PSC, typically made of glass or flexible material, provides mechanical support and stability.
2. Electron Transport Layer (ETL): The ETL is situated on top of the substrate. It facilitates the movement of electrons generated in the perovskite layer. Commonly used materials for the ETL in-plane heterostructure PSCs include titanium dioxide (TiO_2) or other metal oxides.
3. Perovskite Layer: The solar cell's layer that absorbs light is the perovskite layer. The substance used to make it is often a hybrid organic-inorganic metal halide perovskite known as $CH_3NH_3PbI_3$. The perovskite layer absorbs sunlight and produces excited electrons and holes.
4. Hole Transport Layer (HTL): The HTL is situated on top of the perovskite layer. It facilitates the transport of the positively charged holes generated in the perovskite layer. Commonly used materials for the HTL include organic small molecules or polymers.
5. Contact/Counter Electrode: On top of the HTL, there is a contact electrode, typically made of a metal like gold, silver, or carbon-based material. This electrode collects the holes generated in the perovskite layer and completes the electric circuit.

The plane heterostructure design offers several advantages for PSCs:

Simplified Fabrication: The planar arrangement of the layers simplifies the fabrication process compared to other device architectures. It allows for easier deposition of the different layers, leading to improved reproducibility and scalability.

Reduced Charge Recombination: The planar heterostructure design minimizes the interfacial defects and defects within the perovskite layer, reducing charge recombination and improving the efficiency of the solar cell.

Enhanced Stability: The plane heterostructure can contribute to the stability of PSCs. The uniform and compact structure helps protect the perovskite layer from moisture, oxygen, and other environmental factors that can degrade its performance.

Tandem Configurations: To increase efficiency, the plane heterostructure can be used in tandem configurations with other solar cell technologies. The planar structure makes multijunction solar cells easier to build and allows for greater integration with other materials and technologies.

It's worth noting that the specific materials and layer thicknesses used in plane heterostructure PSCs can change depending on the research or commercial development. Researchers continue to explore and optimize different device architectures and materials to enhance the performance, stability, and manufacturability of PSCs.

2.2.3 PEROVSKITE LIGHT ABSORBING LAYER

One essential element of PSCs is the layer of perovskite that absorbs light. It is in charge of receiving solar energy and using the photovoltaic effect to transform it into electrical energy. Usually, a hybrid organic-inorganic metal halide perovskite substance makes up the perovskite layer.

The perovskite structure, which distinguishes perovskite materials, is a special crystal structure that has the "general formula ABX_3". The A cation in PSCs is often an organic compound, such as formamidinium (FA) or methylammonium (MA). The B cation is a metal ion, most frequently lead (Pb), although it can also be tin (Sn) or a mixture of the two. A halogen ion, such as I, Br, or Cl , is usually the X anion.

2.2.4 ELECTRON TRANSPORT LAYER

The electron transport layer (ETL) in a PSC has an important role in enhancing the movement of electrons generated in the perovskite layer towards the electrode, thereby contributing to the efficient collection and extraction of electrical current. The ETL is typically positioned between the absorbing layer and the contact electrode. Commonly used materials for the ETL in PSCs are metal oxides such as ZnO and TiO_2. It's crucial to note that the specific choice of ETL material and its properties can vary depending on the specific perovskite material, device architecture, and desired device performance [8].

2.2.5 HOLE TRANSPORT LAYER

The hole transport layer (HTL) in a PSC is an important component that promotes the transport of positively charged holes generated in the absorbing layer towards the contact electrode. The HTL is typically positioned between the absorbing layer and the contact electrode. Various organic small molecules or polymers are commonly used as HTL materials in PSCs. The hole transport layer in a PSC serves the functions like Hole Extraction, Hole Conductivity, Energy Level Alignment, Charge Selectivity, Film Morphology and Thickness. The specific choice of HTL material and its properties can vary depending on factors such as the perovskite material, device architecture, and desired device performance. Scientists continue to explore different materials to optimize the hole transport properties and overall efficiency of PSCs [9].

2.3 WORKING

The working principle of a PSC involves several steps that enable the conversion of sunlight into electrical energy. Here's a simplified overview of the working of a PSC:

- Absorption of Sunlight: The layer of perovskite, responsible for absorbing light, effectively captures photons emitted by sunlight. Thanks to its distinctive characteristics, the perovskite material exhibits exceptional efficiency in capturing a diverse range of photons throughout the solar spectrum.

- Generation of Electron-Hole Pairs: The perovskite material produces electron-hole pairs when light is absorbed by it. The electrons in the material get energy from the photons and are boosted to higher energy levels, leaving behind positively charged holes.

- Charge Separation: The internal electric field of the perovskite layer causes the generated electron-hole pairs to split. While the holes flow in the direction of the HTL, the electrons move in the direction of the ETL.

- Electron Transport: The ETL serves as a route for the electrons to get to the contact electrode. It is commonly constructed of materials like TiO_2 or ZnO. The ETL makes it easier to capture and move electrons efficiently.

- Hole Transport: The HTL, usually made up of organic small molecules or polymers, serves as a passage for the holes to move towards the contact electrode. The HTL facilitates the efficient collection and transport of holes.

- Collection of charges: The charge carriers from both the transport layers reach the metal contact, which is typically made of a conductive material like metal or a conductive polymer. The contact electrode collects the respective charges (electrons or holes) and forms an external circuit for the flow of electrical current.

- External Circuit: All the gathered carriers pass through the external circuit, producing an electrical current that may be utilized to power electronic equipment or kept in a battery for later use.

- Continuous Operation: The PSC operates continuously as long as sunlight is available, continuously generating electron-hole pairs, separating and collecting the charges, and converting solar energy into electrical energy[10–12].

2.4 PROPERTIES

Perovskite solar cells (PSCs) possess several properties, namely:

- High Absorption Coefficient: Perovskite materials have a high absorption coefficient, allowing them to proficiently absorb an extensive range of photons from the solar spectrum. This property enables PSCs to generate a significant amount of electrical current even with a thin active layer.

- Tunable Bandgap: The Eg of perovskite materials is easily tunable, by altering the composition of the A, B, and X elements. This tunability allows researchers to optimize the Eg to match the solar spectrum, thereby maximizing the absorption of sunlight and causing the performance of the device to flourish.

- Strong Light-Matter Interaction: Perovskite materials exhibit a strong interaction with light, resulting in efficient charge generation within the material. Electron-hole pairs are generated, when photons are absorbed, which can be separated and collected to produce electrical current.

- Solution Processability: Perovskite materials may be treated directly from solutions, opening the door to scalable and affordable production processes including solution processing, spin coating, or printing technologies. Potential benefits for PSC manufacture on a wide scale are provided by this solution's processability.

- High Power Conversion Efficiency: Over the past ten years, PSCs have made impressive strides in terms of "power conversion efficiency (PCE)". PCE of this type of photovoltaic cells has risen quickly, surpassing 25% at this time, and competing with conventional solar cell technology.

- Low Energy Payback Time: "Energy Payback Time" can be defined as, time duration that a PV cell takes to produce the energy required for its installation and production. PSCs have an energy payback period that is equivalent to or even less than many other solar cell technologies.

- Versatile Device Architectures: PSCs can be fabricated using various device architectures, such as planar heterostructures, mesoporous structures, and tandem configurations. This versatility allows for flexible design options and potential integration with other solar cell technologies, leading to improved performance and efficiency.

Despite their promising properties, PSCs face challenges related to their steadiness and longevity. The perovskite materials are susceptible to moisture, oxygen, heat, and light-induced degradation, which can impact the long-term performance of the solar cell. Ongoing research focuses on developing plans to boost stability, reproducibility and lifespan of PSCs, to make them more suitable for commercial applications[12–14].

CHAPTER 3

SIMULATIONS AND METHODOLOGY

3.1 SCAPS- 1D

"SCAPS 1D (Solar Cell Capacitance Simulator 1D)" is a software tool used for simulating the electrical characteristics and performance of semiconductor devices, particularly solar cells. It is specifically designed for one-dimensional simulations of solar cells, where the device structure is assumed to have a uniform cross-section along the vertical direction. SCAPS 1D allows researchers and engineers to model and analyze various aspects of solar cells, including their electrical behavior, optical properties, and charge carrier transport. It can provide insights into device performance parameters such as C-V characteristics, Q.E., and I.V. characteristics . The software incorporates detailed physical models and algorithms to simulate the operation of solar cells accurately. It takes into account factors such as material properties, device geometry, energy band diagrams, carrier transport mechanisms, and optical absorption to predict the device's behavior under different operating conditions. SCAPS 1D offers a user-friendly interface that allows users to define the device structure, material properties, and experimental conditions. It supports different types of solar cells, including Si-based, thin-film, and emerging technologies like PSCs. Users can input relevant parameters, perform simulations, and analyze the results to gain insights into the device behavior and optimize the design for improved performance. The simulations performed using SCAPS 1D can help researchers understand the fundamental physics governing solar cell operation, guide the optimization of device parameters, and explore new device architectures. It serves as a valuable tool in the development and characterization of photovoltaic technologies, enabling efficient and economical design processes.

3.2 DESIGNING THE SOLAR CELL IN SCAPS 1D

For creating a perovskite solar cell structure in SCAPS 1D, you will need to define the layer structure, material properties, and device parameters. Here is a general outline of the steps involved in setting up a PSC structure in SCAPS 1D:

1. Open SCAPS 1D: Launch the SCAPS 1D software on your computer.

2. Define Layers: Define the layers of your cell structure. In this section we can define our cell structure, order of different layers and metal contacts.

3. Set Material Properties: Specify the material properties for each layer. This includes parameters such as bandgap, carrier mobility, doping concentration, and thickness. You will need to input the relevant material properties for the perovskite material, ETL, HTL, and any other layers in your structure.

4. Set Device Parameters: Define the device parameters for your PV cell. This includes factors like temperature, incident light intensity, and applied voltage. You may also need to specify other device-specific parameters like contact resistances or interface properties.

5. Choose Simulation Method: Select the appropriate simulation method for your analysis. SCAPS 1D offers various simulation techniques, including steady-state, transient, and frequency-domain simulations. Choose the method that suits your specific analysis requirements.

6. Run Simulation: Run the simulation in SCAPS 1D based on your defined structure, material properties, and device parameters. The software will calculate the electrical characteristics of your PSC, such as current-voltage (I-V) curves, quantum efficiency, or capacitance-voltage (C-V) characteristics.

7. Analyze Results: Once the simulation is complete, analyze the results obtained from SCAPS 1D. This may involve studying the device's performance, optimizing parameters, comparing different structures, or extracting relevant figures of merit.

Setting parameters in SCAPS 1D involves defining the material properties, layer structure, device parameters, and simulation settings. Here is a general guide on how to set parameters in SCAPS 1D:

1. Material Properties:
   - Open the material database in SCAPS 1D.

- Specify the relevant material properties for each layer in your solar cell structure, such as bandgap, effective mass, carrier mobility, doping concentration, and trap densities.

- You can select the materials from the built-in database or add new materials if required.

2. Layer Structure:

- Define the layer structure of your solar cell by specifying the number of layers and their respective thicknesses.

- Assign the materials to each layer based on the material properties defined in step 1.

- Specify the doping profiles, if applicable.

3. Device Parameters: To set device parameters in SCAPS 1D for your solar cell simulation, follow these steps:

- Open SCAPS 1D: Launch the SCAPS 1D software on your computer.

- Define Layer Structure and Material Properties: Set up the layer structure and specify the material properties for each layer in your solar cell. This includes the substrate, electron transport layer (ETL), perovskite layer, hole transport layer (HTL), and contact electrode. Refer to the material database in SCAPS 1D to input the appropriate material properties for each layer.

- Set Temperature: Specify the temperature at which you want to simulate your solar cell. This parameter affects various material properties, carrier mobilities, and recombination rates within the device.

- Define Incident Light Intensity: Input the incident light intensity in the simulation. This parameter represents the intensity of light irradiating on the solar cell and affects the amount of generated photocurrent.

- Specify Applied Voltage: Set the applied voltage or bias across the solar cell. This parameter determines the external electrical field within the device and affects the current-voltage (I-V) characteristics.

- Define Contacts and Interface Properties: Specify the electrical contacts and their properties. This includes parameters such as contact resistances, work functions, and

barrier heights. Properly defining the contacts is crucial for accurately simulating the charge carrier transport and extraction within the solar cell.

- Set Trap Properties (optional): If you are studying trap-assisted processes within the solar cell, you can define trap properties, such as trap densities, capture cross-sections, and emission rates. This step is optional and depends on the specific analysis you want to perform.

- Choose Simulation Method and Settings: Select the appropriate simulation method, such as steady-state or transient, based on your analysis requirements. Set the simulation time or frequency range, numerical algorithms, and convergence criteria.

- Run Simulation: Start the simulation in SCAPS 1D. The software will calculate the electrical characteristics of your solar cell based on the defined device parameters.

- Analyze Results: Once the simulation is complete, analyze the results obtained from SCAPS 1D. Plot and evaluate relevant characteristics such as current-voltage (I-V) curves, quantum efficiency, or capacitance-voltage (C-V) characteristics [15].

3.3 SIMULATION FOR NUMERICAL ANALYSIS OF CsGeBr$_3$

The photovoltaic device studied has the following components: Ag (metal back contact)/CuSCn (HTL)/CsGeBr$_3$ (absorbing layer)/C$_{60}$(ETL)/FTO. Fig 3.1 depicts the construction of the aforementioned cell structure. Table 3.1 presents the distinctive factors of CsGeBr$_3$, CuSCN, FTO, and C$_{60}$, which were obtained from a variety of theoretical and experimental studies that have been published in the press [16–20]. A Eg of 2.33eV indicates the outstanding effectiveness of solar cells of CsGeBr$_3$ [17]. It is supposed that the thermal velocities of electrons and holes for all the elements used in the cell are 10^7 cm.s^{-1}, respectively. The work functions for FTO and Ag are presumed to be 3.5 eV and 4.78 eV, respectively.
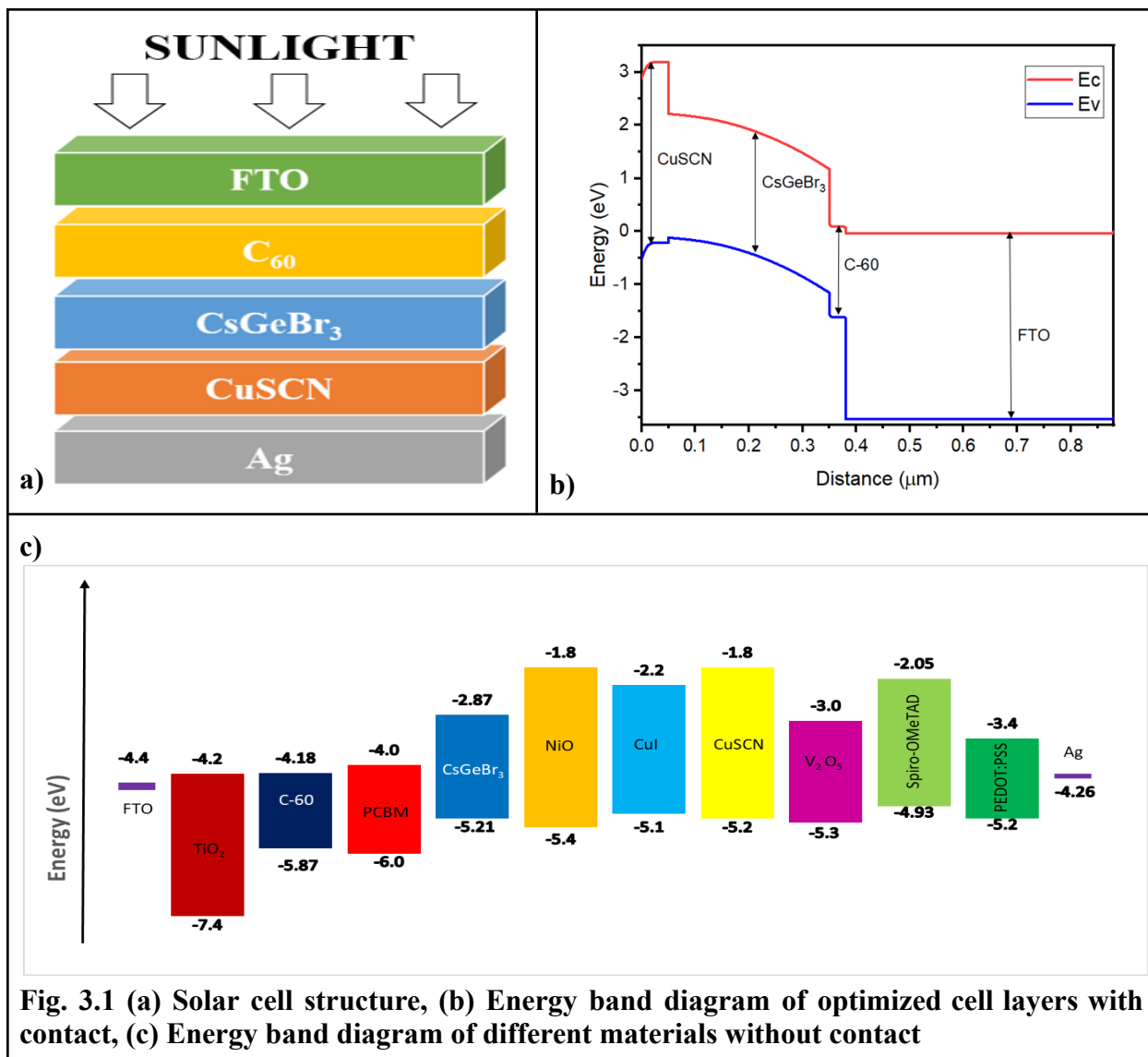
Fig. 3.1 (a) Solar cell structure, (b) Energy band diagram of optimized cell layers with contact, (c) Energy band diagram of different materials without contact

Table 3.1 Parameters for material used in this simulation.

Parameters	FTO	C_{60}	$CsGeBr_3$	CuSCN
Thickness(nm)	500	30	3000	50
E_g (eV)	3.5	1.7	2.33	3.4
Electron affinity(eV)	4	3.9	2.87	1.9
Permittivity	9	4.2	3.9	10
N_c (cm^{-3})	2.2×10^{18}	8×10^{19}	1.9×10^{18}	1.7×10^{19}
N_v (cm^{-3})	1.8×10^{19}	8×10^{19}	2.07×10^{18}	2.5×10^{21}
Electron Mobility	20	100	20	10^{-4}
Hole Mobility	10	2.5×10^3	20	10^{-1}
N_D (cm^{-3})	10^{19}	0	0	0
N_A (cm^{-3})	0	2.6×10^{18}	2×10^{16}	10^{18}
Defect density (cm^{-3})	10^{13}	10^{13}	10^{13}	10^{13}

CHAPTER 4

RESULTS AND DISCUSSION

4.1 INFLUENCE OF ABSORBER LAYER THICKNESS, $CsGeBr_3$

The "thickness of the absorber layer" in a perovskite solar cell has a prominent command on its execution. Here are some effects of modifying the thickness of the absorber layer:

- Optical Absorption: The size of the absorber layer has a direct impact on how much light it can absorb. More light may be absorbed by an absorber layer if it is thicker, which leads to more electron-hole pairs being produced. At the front and rear interfaces, significant light reflection and absorption losses can also be caused by absorber layers that are too thick.

- Charge Carrier Collection: The produced charge carriers' journey distance to the ETL and HTL depends on the width of the absorber layer. Probability of charge carriers recombining before being collected may rise if the absorber layer is excessively thick. However, a very thin absorber layer might not be able to create and trap enough charge carriers.

- Short-Circuit Current (J_{SC}): It is the maximum current produced by a solar cell, and it is directly influenced by the width of the perovskite layer. The J_{SC} typically rises up to a certain point when the absorber layer thickness is increased, after which it plateaus or falls because of higher recombination losses.

- Open-Circuit Voltage (V_{OC}): The absorber layer thickness can have an impact on the V_{OC}, which is the maximal voltage generated by a solar cell. Due to an increase in trap-assisted recombination or a higher density of states, thickening the perovskite layer occasionally results in a diminishment of V_{OC}.

- F.F. (F.F.): F.F. is a measurement of the cell's capacity to convert light into electrical current. A greater F.F., indicating effective charge carrier collection and lower losses, might be the outcome of an appropriate thickness.

- Power Conversion Efficiency (PCE): Overall performance of a PSC is majorly affected by thickness of absorber layer. Light absorption, charge carrier production, collection, and recombination losses may all be balanced at an ideal thickness. Reduced PCE might happen if the thickness is not maintained.

- Optimizing the absorber layer thickness in a PSC is crucial to achieving the best balance between light absorption, charge carrier generation, and collection. Different device architectures and material compositions may have different optimal thickness ranges, and it often requires experimental and computational investigations to determine the ideal absorber layer thickness for a specific PSC design[21].
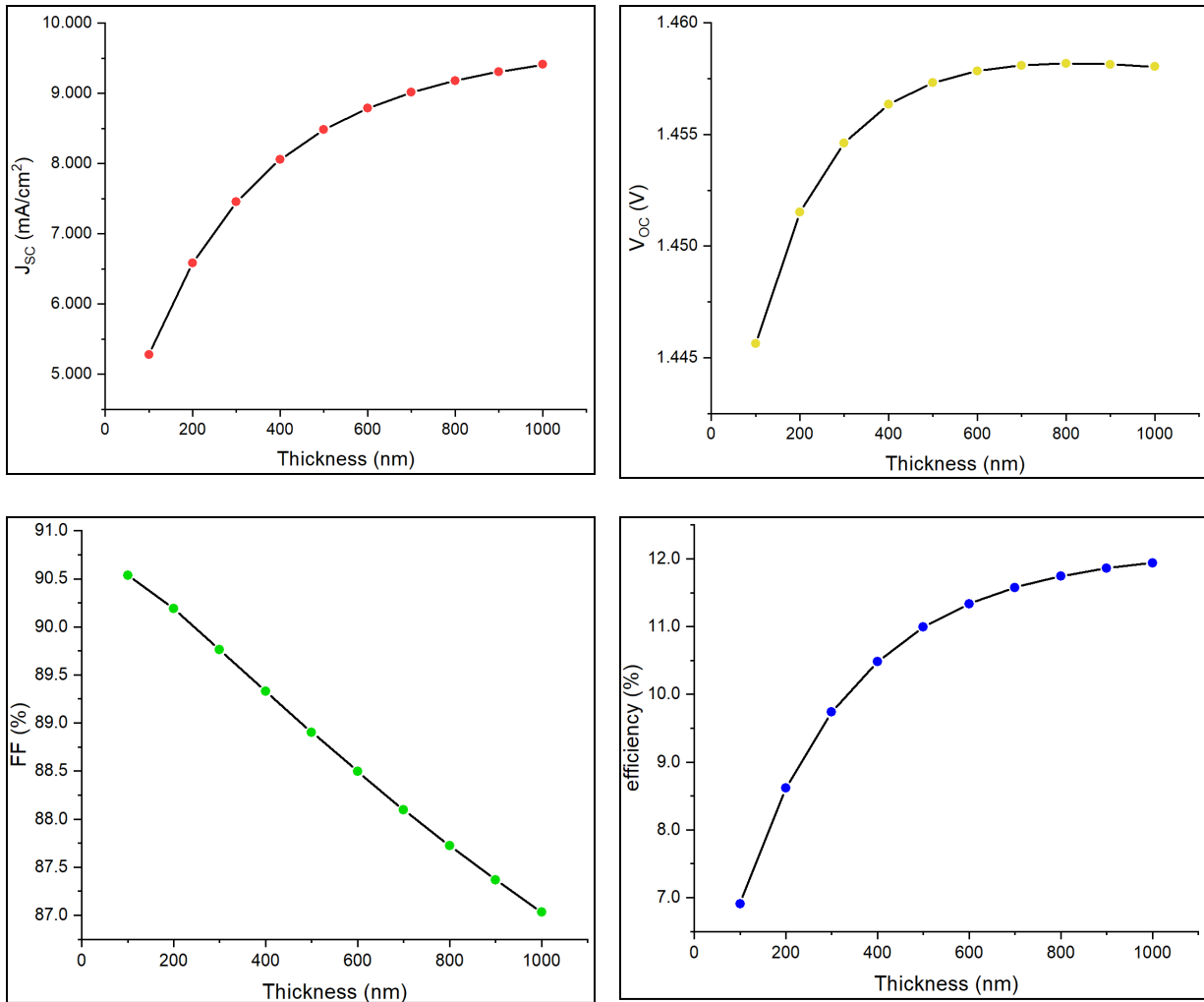
Fig. 4.1 Alteration in device characteristics due to modification in thickness of absorber layer.

When simulations are carried out for optimizing the absorber layer width by changing it from 0.1μm to 1 μm. We observe, the thickness increases along with the increment in current density. It reaches its maximum value of 8.788 Am/cm^2 as the thickness reaches 0.6 μm. This suggests that a larger absorber layer may absorb more photons and, as a result, can provide excess charge carrier concentration at longer wavelengths, which facilitates the formation of electron-hole pairs as illustrated in Fig. 4.1a. According to Fig. 4.1b, an increase in thickness has an impact on V_{OC} values; initially, the V_{OC} slightly rises before becoming almost constant as the thickness rises more and the number of stars decreases. As seen in Fig. 4.1c, the F.F. falls as the layer becomes thicker. The PCE of the device rises with the extension in thickness, as shown in Fig. 4.1d, and reaches a high of 11.3% at 0.6 μm. With higher charge carrier concentration and more light

absorption as a result of increased thickness, J_{SC} values rise due to the material's extremely high absorption coefficient of Ge-based perovskites (up to 105 cm^{-1}) [22].

4.2 INFLUENCE OF TEMPERATURE OF CsGeBr$_3$ PSC

The temperature at which a solar cell operates is significantly responsible for its performance. The simulation was run with temperatures ranging from 305 K to 423 K, and it was discovered that 326 K was the ideal temperature when analyzed with a continuous light of 1000 W/m^2. Higher temperatures will have an impact on material properties like carrier concentration, band gap energies, and mobility of electrons and holes, which will impair cell efficiency[23]. The impact of temperature on J_{SC}, V_{OC}, F.F., and PCE is displayed in Fig. 4.2. As illustrated in the figure that a rise in temperature causes the V_{OC} to fall. Consequently, the influence of operating temperature on current density is negligible because of the unavoidable drop in voltage. The F.F. is shown to first rise with temperature before sharply falling. At the point where the perovskite layer is 0.6 μm thick and the temperature is 305 K, the F.F and PCE are at their highest values. This shows the characteristics of the cell with a 2.33 band gap and a 0.6 μm absorber, such as V_{OC}, F.F., , J_{SC} and PCE, with temperatures varying from 305 K to 423 K [24–27].
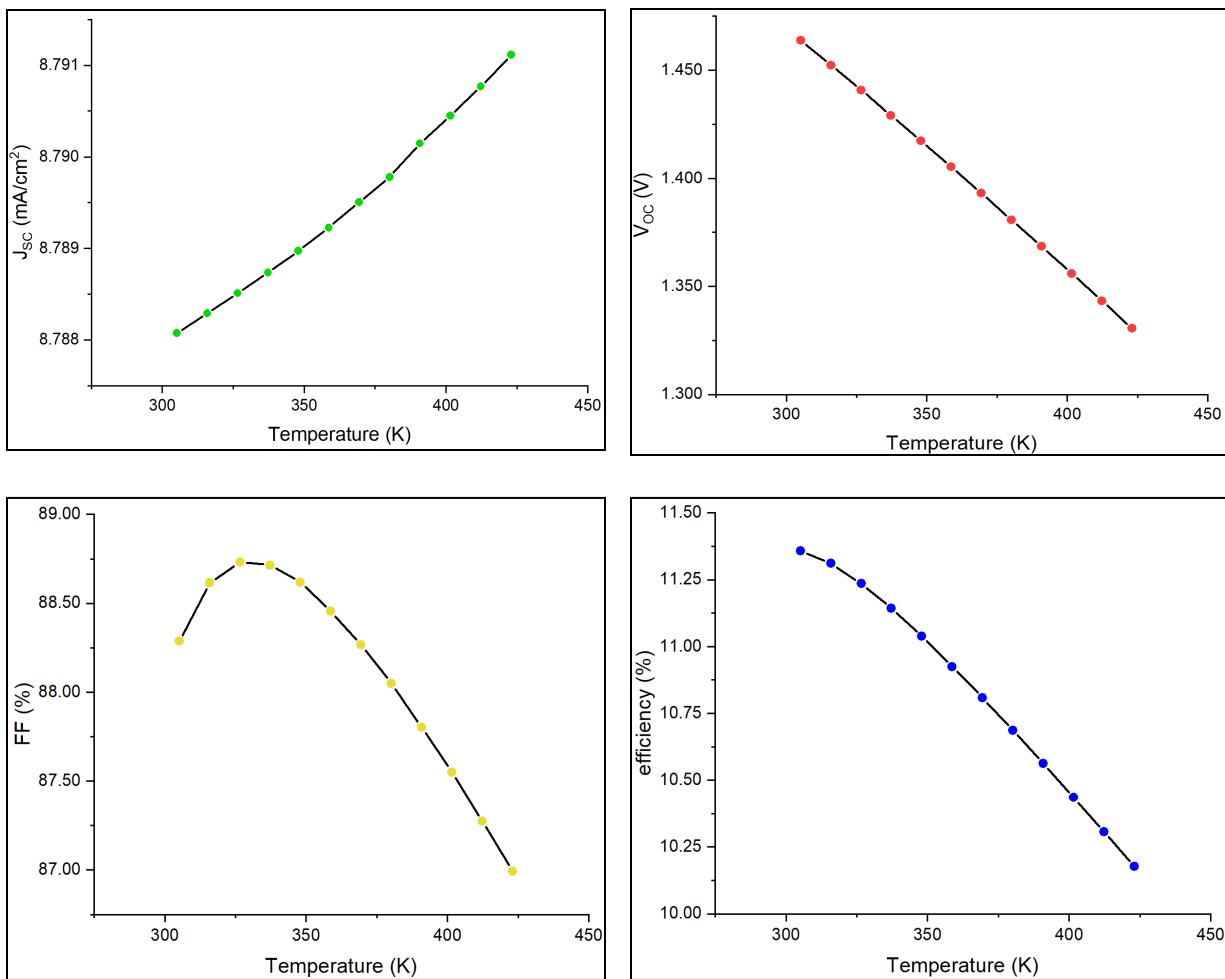
Fig.4.2 Alteration in device characteristics due to modification in Temperature.

4.3 INFLUENCE OF DEFECT DENSITY OF ABSORBER LAYER, CsGeBr$_3$

The defect density in the absorbing layer of a PSC can have a prominent impact on its effectiveness. Defects in the absorbing layer can induce trap-assisted recombination, which affects the V_{OC} of the solar cell. Traps capture and release charge carriers, leading to a loss in the voltage potential across the device. Higher N_t often results in lower V_{OC} due to increased trap-assisted recombination. Defects can also impact the F.F. of the PSC. Excessive N_t can introduce additional resistive and recombination losses, reducing the F.F. This leads to a decrease in the overall current collection and power output of the solar cell. Defects can contribute to the instability and degradation of PSCs. They can facilitate various degradation mechanisms, such as ion migration, moisture ingress, and phase segregation, leading to reduced device performance and lifespan. For producing high-performance PSCs, the N_t in the absorbing layer must be controlled and reduced. Researchers and engineers employ various strategies, such as optimizing the fabrication processes, passivating defect sites, and improving the material quality, to reduce the N_t and enhance the device performance. Additionally, advanced characterization techniques are used to study and quantify the governance of defects on electrical and optical properties of PSCs [28–30].
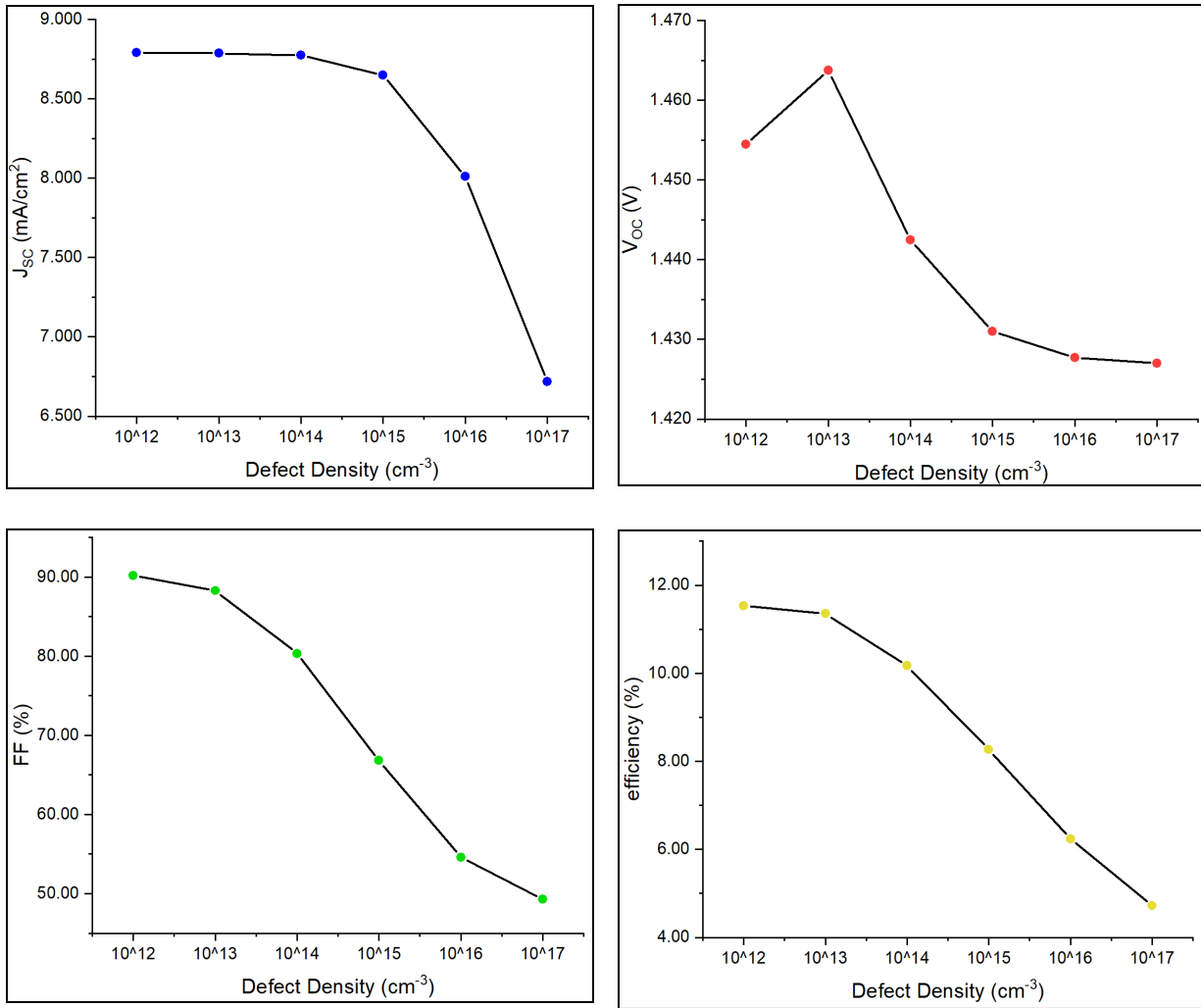
Fig. 4.3 Alteration in device characteristics due to modification in Defect Density of absorber layer.

The defect density notably influences the productivity of the solar cell in the perovskite layer. Fig. 4.3 shows how N_t affects every parameter (J_{SC}, V_{OC}, F.F. and PCE). The graph shows that the value of J_{SC} first appears to be practically constant before falling. While the V_{OC} initially rises, then falls, and eventually remains steady. With a rise in the absorber layer's N_t, the F.F. similarly drops. We conclude that the efficiency is directly influenced by N_t because as defects multiply, charge carriers' diffusion lengths shorten and recombination carriers accumulate in the absorber layer. 10^{13} is found to be the ideal N_t of the proposed solar cell.

4.4 COMPARISON OF DIFFERENT ETL AND HTL COMBINATIONS

Cell performance for different cell structures was studied by varying ETL and HTL layers. Fig. 4.4 and 4.5 indicates J-V and Q-E characteristics with different HTL and ETL materials, respectively. "Table 4.1 demonstrates the PCE(%) of the solar cell with the different materials used as ETLs and HTLs". The table clearly demonstrates that when different ETL and HTL layers are used, the combination of C_{60} (ETL) and CuSCN (HTL) yields the most promising results in terms of cell performance.

(a)

(b)
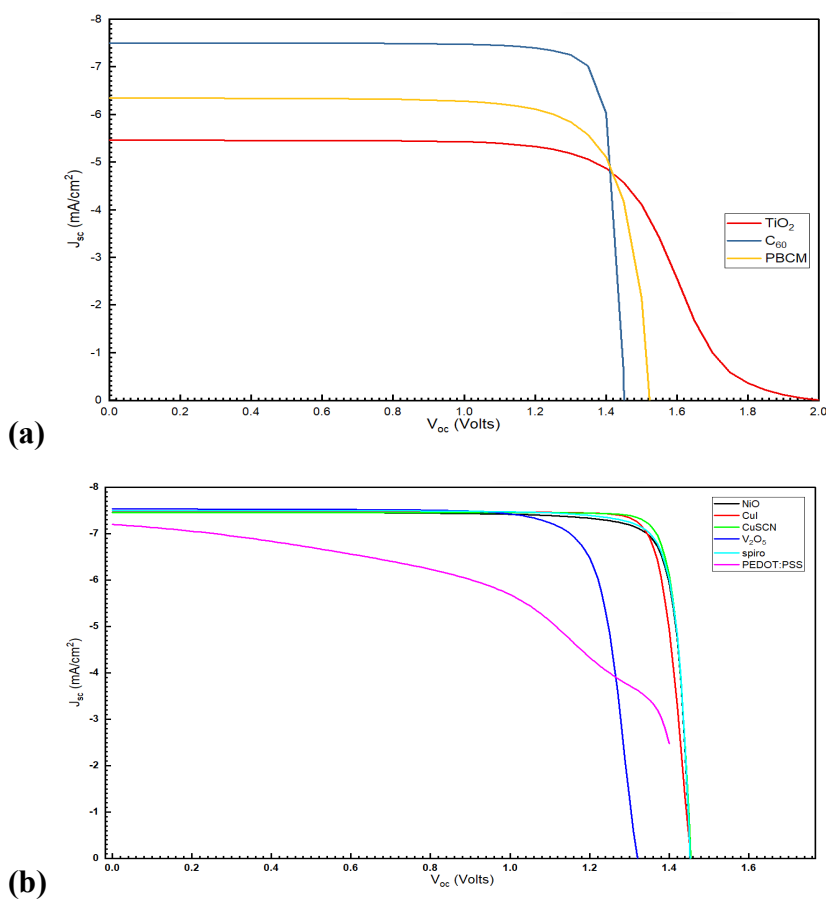
Fig. 4.4 J-V characteristics of different (a) ETL and (b) HTL materials.

Table 4.1 Performance of solar cells employing different combinations of various elements as ETL and HTL.

Cell structures	J_{SC} (mA/cm^2)	V_{OC} (V)	F.F. (%)	PCE (%)
Ag/NiO/CsGeBr$_3$/TiO$_2$/FTO	5.402	1.895	66.02	6.76
Ag/CuI/CsGeBr$_3$TiO$_2$/FTO	5.415	1.982	67.90	7.29
Ag/CuSCN/CsGeBr$_3$/TiO$_2$/FTO	5.402	2.150	63.64	7.39
Ag/V$_2$O$_5$/CsGeBr$_3$/TiO$_2$/FTO	5.498	1.592	64.82	5.68
Ag/Spiro-OMeTAD/CsGeBr$_3$/TiO$_2$/FTO	5.455	1.878	66.77	6.84
Ag/PEDOT:PSS/CsGeBr$_3$/TiO$_2$/FTO	5.060	1.561	40.17	3.17
Ag/NiO/CsGeBr$_3$/C$_{60}$/FTO	7.456	1.452	86.99	9.42
Ag/CuI/CsGeBr$_3$/C$_{60}$/FTO	7.465	1.454	88.15	9.57
Ag/CuSCN/CsGeBr$_3$/C$_{60}$/FTO	7.455	1.454	89.77	9.74
Ag/V$_2$O$_5$/CsGeBr$_3$/C$_{60}$/FTO	7.532	1.319	81.05	8.06
Ag/Spiro-OMeTAD/CsGeBr$_3$/C$_{60}$/FTO	7.497	1.452	87.25	9.50
Ag/PEDOT:PSS/CsGeBr$_3$/C$_{60}$/FTO	7.199	1.475	53.81	5.72
Ag/NiO/CsGeBr$_3$/PCBM/FTO	6.298	1.540	77.72	7.54
Ag/CuI/CsGeBr$_3$/PCBM/FTO	6.308	1.54	82.18	7.98
Ag/CuSCN/CsGeBr$_3$/PCBM/FTO	6.298	1.550	83.06	8.11
Ag/V$_2$O$_5$/CsGeBr$_3$/PCBM/FTO	6.298	1.54	77.72	7.54
Ag/Spiro-OMeTAD/CsGeBr$_3$/PCBM/FTO	6.340	1.539	77.88	7.60
Ag/PEDOT:PSS/CsGeBr$_3$/PCBM/FTO	5.751	1.759	36.83	3.73
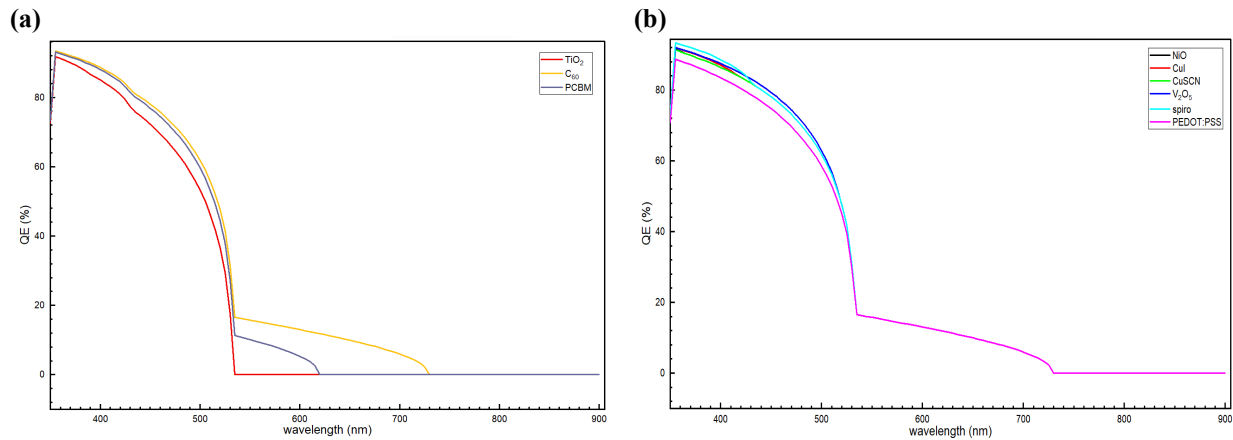
Fig. 4.5 Quantum Efficiency QE (%) curve of different (a) ETL and (b) HTL materials.

The efficiency of a solar cell that utilizes perovskite light absorbers made of germanium is greatly influenced by the absorber layer. Temperature variations, N_t and the thickness of the perovskite layer all have considerable repercussions on the functionality of solar cells. They should be optimized to bring photogenerated electrons and holes into equilibrium, using the names absorption and mixing [31]. First, the absorber layer width is increased from 0.1**μ**m to 1**μ**m. We then improved the cell by raising its temperature from 273 K to 423 K using the measurement fit we found. Next, we changed the N_t of the active layer from 10^{12} cm^{-3} to 10^{17} cm^{-3} to get the ideal temperature and thickness of CsGeBr$_3$. We modeled the absorber layer thickness, flaws, and cell temperature effects on the photovoltaic performance of a Ge-based PSC with a 2.33 eV energy gap. The properties of the device include PCE, F.F., J$_{SC}$, and V$_{OC}$.

CHAPTER 5

CONCLUSION

We investigated the impact of different ETLs and HTLs affecting PSCs and inferred that C_{60} as the ETL and CuSCN as the HTL is the most befitting combination. We have investigated how multiple factors, such as operating temperature, absorber layer thickness and N_t, affect device characteristics, using the SCAPS-1D simulator programme. The simulation result has shown that the maximum PCE of 11.35% has been attained for the device structure Ag/CuSCN/CsGeBr$_3$/C$_{60}$/FTO for 600 nm thickness. The optimized value of temperature and N_t of the PSC is 305 K and 10^{13} units respectively. We discover that the effectiveness found in the simulated results is 9.74% using perovskite quantum rods, whereas it is 4.92% in the literature. When we compare our findings with the results from the literature. We utilized C_{60} as an ETL in our suggested structure because of its improved electron transporting capabilities, reduction of hysteresis, and low-temperature processing. It can also be packed more tightly to improve inter-molecular charge transmission in addition to these characteristics [32–34]. On the other hand, the use of CuSCN as the HTL in the structure is attributed to its natural thermal stability, exceptional resistance to high temperatures, and extremely durable crystalline structure. Furthermore, its band alignment with the perovskite is perfect [35–37]. Additionally, the PCE of the outcome has significantly improved in the optimized findings. When compared to the literature - reported experimental measurements, the result of the original calculation and the optimized results obtained in this paper.

REFERENCES

[1] A. J. Curran *et al.*, "Degradation of PERC and Al-BSF Cells with UV Cutoff and White Variations of EVA and POE Encapsulant," *Conference Record of the IEEE Photovoltaic Specialists Conference*, pp. 1510–1516, Jun. 2021, doi: 10.1109/PVSC43889.2021.9519110.

[2] C. Becker *et al.*, "Polycrystalline silicon thin-film solar cells: Status and perspectives," *Solar Energy Materials and Solar Cells*, vol. 119, pp. 112–123, 2013, doi: 10.1016/j.solmat.2013.05.043.

[3] R. Goswami, "Three Generations of Solar Cells," *Adv Mat Res*, vol. 1165, pp. 113–130, Jul. 2021, doi: 10.4028/WWW.SCIENTIFIC.NET/AMR.1165.113.

[4] M. A. Green *et al.*, "Solar cell efficiency tables (Version 53)," *Progress in Photovoltaics: Research and Applications*, vol. 27, no. 1, pp. 3–12, Jan. 2019, doi: 10.1002/PIP.3102.

[5] D. Zhou, T. Zhou, Y. Tian, X. Zhu, and Y. Tu, "Perovskite-Based Solar Cells: Materials, Methods, and Future Perspectives," *J Nanomater*, vol. 2018, 2018, doi: 10.1155/2018/8148072.

[6] A. Raj, M. Kumar, H. Bherwani, A. Gupta, and A. Anshul, " Evidence of improved power conversion efficiency in lead-free CsGeI 3 based perovskite solar cell heterostructure via scaps simulation ," *Journal of Vacuum Science & Technology B*, vol. 39, no. 1, p. 012401, Jan. 2021, doi: 10.1116/6.0000718/591372.

[7] R. Wang, M. Mujahid, Y. Duan, Z. K. Wang, J. Xue, and Y. Yang, "A Review of Perovskites Solar Cell Stability," *Adv Funct Mater*, vol. 29, no. 47, p. 1808843, Nov. 2019, doi: 10.1002/ADFM.201808843.

[8] K. Mahmood, S. Sarwar, and M. T. Mehran, "Current status of electron transport layers in perovskite solar cells: materials and properties," *RSC Adv*, vol. 7, no. 28, pp. 17044–17062, Mar. 2017, doi: 10.1039/C7RA00002B.

[9] W. Tress, N. Marinova, O. Inganas, M. K. Nazeeruddin, S. M. Zakeeruddin, and M. Graetzel, "The role of the hole-transport layer in perovskite solar cells - Reducing recombination and increasing absorption," *2014 IEEE 40th Photovoltaic Specialist Conference, PVSC 2014*, pp. 1563–1566, Oct. 2014, doi: 10.1109/PVSC.2014.6925216.

[10] N. Marinova, S. Valero, and J. L. Delgado, "Organic and perovskite solar cells: Working principles, materials and interfaces," *J Colloid Interface Sci*, vol. 488, pp. 373–389, Feb. 2017, doi: 10.1016/J.JCIS.2016.11.021.

[11] I. Mora-Seró, "How Do Perovskite Solar Cells Work?," *Joule*, vol. 2, no. 4, pp. 585–587, Apr. 2018, doi: 10.1016/J.JOULE.2018.03.020.

[12] N. G. Park, "Perovskite solar cells: an emerging photovoltaic technology," *Materials Today*, vol. 18, no. 2, pp. 65–72, Mar. 2015, doi: 10.1016/J.MATTOD.2014.07.007.

[13] T. Bin Song *et al.*, "Perovskite solar cells: film formation and properties," *J Mater Chem A Mater*, vol. 3, no. 17, pp. 9032–9050, Apr. 2015, doi: 10.1039/C4TA05246C.

[14] Y. Chen *et al.*, "Improved optical properties of perovskite solar cells by introducing Ag nanopartices and ITO AR layers," *Scientific Reports 2021 11:1*, vol. 11, no. 1, pp. 1–9, Jul. 2021, doi: 10.1038/s41598-021-93914-1.

[15] M. Burgelman, K. Decock, A. Niemegeers, J. Verschraegen, and S. Degrave, "SCAPS manual," *users.elis.ugent.be*, Accessed: May 23, 2023. [Online]. Available: https://users.elis.ugent.be/ELISgroups/solar/projects/scaps/SCAPS%20manual%20most%20recent.pdf

[16] K. Chakraborty, M. G. Choudhury, and S. Paul, "Numerical study of Cs2TiX6 (X = Br−, I−, F− and Cl−) based perovskite solar cell using SCAPS-1D device simulation," *Solar Energy*, vol. 194, pp. 886–892, Dec. 2019, doi: 10.1016/J.SOLENER.2019.11.005.

[17] U. G. Jong, C. J. Yu, Y. H. Kye, Y. G. Choe, W. Hao, and S. Li, "First-Principles Study on Structural, Electronic, and Optical Properties of Inorganic Ge-Based Halide Perovskites," *Inorg Chem*, vol. 58, no. 7, pp. 4134–4140, Apr. 2019, doi: 10.1021/ACS.INORGCHEM.8B03095.

[18] U. Schwarz, F. Wagner, K. Syassen, and H. Hillebrecht, "Effect of pressure on the optical-absorption edges of and," *Phys Rev B Condens Matter Mater Phys*, vol. 53, no. 19, pp. 12545–12548, 1996, doi: 10.1103/PHYSREVB.53.12545.

[19] D. Saikia, M. Alam, J. Bera, A. Betal, A. N. Gandi, and S. Sahu, "A First-Principles Study on ABBr3 (A = Cs, Rb, K, Na; B = Ge, Sn) Halide Perovskites for Photovoltaic Applications," *Adv Theory Simul*, vol. 5, no. 12, Dec. 2022, doi: 10.1002/ADTS.202200511.

[20] U. Jonga, C. Yu, Y. Kye, Y. Choe, … H. W. preprint arXiv, and undefined 2018, "Structural and optoelectronic properties of the inorganic perovskites AGeX3 (A= Cs, Rb; X= I, Br, Cl) for solar cell application," *arxiv.org*, 2018, Accessed: Apr. 03, 2023. [Online]. Available: https://arxiv.org/abs/1810.02543

[21] A. Bag, R. Radhakrishnan, R. Nekovei, and R. Jeyakumar, "Effect of absorber layer, hole transport layer thicknesses, and its doping density on the performance of perovskite solar cells by device simulation," *Solar Energy*, vol. 196, pp. 177–182, Jan. 2020, doi: 10.1016/J.SOLENER.2019.12.014.

[22] P. P. Sun, Q. S. Li, L. N. Yang, and Z. S. Li, "Theoretical insights into a potential lead-free hybrid perovskite: Substituting Pb2+ with Ge2+," *Nanoscale*, vol. 8, no. 3, pp. 1503–1512, Jan. 2016, doi: 10.1039/C5NR05337D.

[23]   T. Nakada and M. Mizutani, "18% efficiency Cd-free Cu(In, Ga)Se2 thin-film solar cells fabricated using chemical bath deposition (CBD)-ZnS buffer layers," *Japanese Journal of Applied Physics, Part 2: Letters*, vol. 41, no. 2 B, Feb. 2002, doi: 10.1143/JJAP.41.L165.

[24]   G. Liu *et al.*, "Dependence of power conversion properties of perovskite solar cells on operating temperature," *Appl Phys Lett*, vol. 113, no. 11, Sep. 2018, doi: 10.1063/1.5041028.

[25]   Q. Meng *et al.*, "Effect of temperature on the performance of perovskite solar cells," *Journal of Materials Science: Materials in Electronics*, vol. 32, no. 10, pp. 12784–12792, May 2021, doi: 10.1007/S10854-020-03029-Y.

[26]   H. Zhang, X. Qiao, Y. Shen, and M. Wang, "Effect of temperature on the efficiency of organometallic perovskite solar cells," *Journal of Energy Chemistry*, vol. 24, no. 6, pp. 729–735, Nov. 2015, doi: 10.1016/j.jechem.2015.10.007.

[27]   P. Roy, N. K. Sinha, and A. Khare, "An investigation on the impact of temperature variation over the performance of tin-based perovskite solar cell: A numerical simulation approach," *Mater Today Proc*, vol. 39, pp. 2022–2026, 2019, doi: 10.1016/j.matpr.2020.09.281.

[28]   S. Mahjabin *et al.*, "Perceiving of Defect Tolerance in Perovskite Absorber Layer for Efficient Perovskite Solar Cell," *IEEE Access*, vol. 8, pp. 106346–106353, 2020, doi: 10.1109/ACCESS.2020.3000217.

[29]   Shubham, Raghvendra, C. Pathak, and S. K. Pandey, "Design, Performance, and Defect Density Analysis of Efficient Eco-Friendly Perovskite Solar Cell," *IEEE Trans Electron Devices*, vol. 67, no. 7, pp. 2837–2843, Jul. 2020, doi: 10.1109/TED.2020.2996570.

[30]   T. Ouslimane, L. Et-taya, L. Elmaimouni, and A. Benami, "Impact of absorber layer thickness, defect density, and operating temperature on the performance of MAPbI3 solar cells based on ZnO electron transporting material," *Heliyon*, vol. 7, no. 3, Mar. 2021, doi: 10.1016/j.heliyon.2021.e06379.

[31]   P. Zhao *et al.*, "Device simulation of inverted CH3NH3PbI3−xClx perovskite solar cells based on PCBM electron transport layer and NiO hole transport layer," *Solar Energy*, vol. 169, pp. 11–18, Jul. 2018, doi: 10.1016/J.SOLENER.2018.04.027.

[32]   X. Liu *et al.*, "Novel efficient C60-based inverted perovskite solar cells with negligible hysteresis," *Electrochim Acta*, vol. 288, pp. 115–125, Oct. 2018, doi: 10.1016/J.ELECTACTA.2018.09.004.

[33]   H. Zhou, J. Mei, M. Xue, Z. Song, and H. Wang, "High-stability, self-powered perovskite photodetector based on a CH3NH3PbI3/GaN heterojunction with C60 as an electron transport layer," *Journal of Physical Chemistry C*, vol. 121, no. 39, pp. 21541–21545, Oct. 2017,   doi: 10.1021/ACS.JPCC.7B07536/ASSET/IMAGES/LARGE/JP-2017-075366_0006.JPEG.

[34] C. Xu *et al.*, "Comparative Study on TiO2and C60Electron Transport Layers for Efficient Perovskite Solar Cells," *ACS Appl Energy Mater*, vol. 4, no. 6, pp. 5543–5553, Jun. 2021, doi: 10.1021/ACSAEM.1C00226/ASSET/IMAGES/LARGE/AE1C00226_0009.JPEG.

[35] M. Jung *et al.*, "Thermal Stability of CuSCN Hole Conductor-Based Perovskite Solar Cells," *ChemSusChem*, vol. 9, no. 18, pp. 2592–2596, Sep. 2016, doi: 10.1002/CSSC.201600957.

[36] B. Mahapatra, R. V. Krishna, Laxmi, and P. K. Patel, "Design and optimization of CuSCN/CH3NH3PbI3/TiO2 perovskite solar cell for efficient performance," *Opt Commun*, vol. 504, Feb. 2022, doi: 10.1016/J.OPTCOM.2021.127496.

[37] A. Nizamuddin, F. Arith, I. J. Rong, M. Zaimi, A. S. Rahimi, and S. Saat, "Investigation of Copper(I)Thiocyanate (CuSCN) as a Hole Transporting Layer for Perovskite Solar Cells Application," *Journal of Advanced Research in Fluid Mechanics and Thermal Sciences*, vol. 78, no. 2, pp. 153–159, Feb. 2021, doi: 10.37934/ARFMTS.78.2.153159.

Plagiarism Report

Dr. Sarita Baghel

SUPERVISOR

44

45

Registration Proof

Paytm

Payment Successful

₹2,000 ✅

Rupees Two Thousand Only

To: **Registrar Nsut Wss**
Union Bank of India

From: Anushansha Yadav
Union Bank of India - 5802

UPI Ref. No: 3114130 **98511**
10:44 AM, 24 Apr 2023

POWERED BY
UPI
UNIFIED PAYMENTS INTERFACE

Acceptance Record

2 messages

International Conference <icamet@nsut.ac.in>   Sun, Apr 16, 2023 at 10:26 AM
To: icamet@nsut.ac.in
Bcc: anuy9168@gmail.com

Dear   Madam/Sir,

Greetings!!

Thank you for the interest shown in ICAMET-2023 and submitting your abstract for presentation. I am pleased to inform you that **Abstract of your paper has been accepted** for presentation during the International Conference on Advanced Materials for Emerging Technologies (ICAMET-2023) to be held at APJ-11, Netaji Subhas University of Technology, New Delhi.

You are requested to complete the registration process by paying the registration fee as per details available on conference website: www.icamet.in

We look forward to welcoming you at Netaji Subhas University of Technology, New Delhi, India.

Thanking you,

Organizing Committee
ICAMET-2023
Website: www.icamet.in
Email: icamet@nsut.ac.in

RESEARCH PAPER

Investigating the efficiency and optimizing of Germanium-based Perovskite Solar Cell using SCAPS 1D

Anushansha Yadav, Vanshika, Rahul Kundara, Sarita Baghel
[1,2,3,4]*Department of Applied Physics, Delhi Technological University, Shahbad Daulatpur, Main Bawana Road, Delhi, India
E-mail: anuy9168@gmail.com

1. ABSTRACT

The Germanium-based perovskite solar cell (PSC) is a viable alternative to traditional lead-based PSCs, as it is not hazardous to the environment. To investigate this, simulations were conducted using various Hole Transport Layers (HTLs) and Electron Transport Layers (ETLs). Factors such as absorber layer thickness, operating temperature, and defect density were analyzed using SCAPS-1D. The simulations revealed that CuSCN and C_{60} were suitable for HTL and ETL, respectively. With a thickness of 600 nm of absorber layer at 305 K, the device achieved a maximum PCE of 11.35%. The solar devices showed stability at 305 K, based on the photovoltaic parameters. Therefore, the $CsGeBr_3$ PSC is a promising device for future photovoltaic applications and for designing highly efficient lead-free PSCs.

2. INTRODUCTION

Solar energy has emerged as a highly viable alternative to the energy derived from non-renewable sources in today's society, which is moving toward eco-friendly alternatives for everything. Solar cells are the gadgets that use the photoelectric effect to convert direct sunlight into electric energy.[1] As a third-generation photovoltaic technology, PSCs have gained prominence because of its advantages of low production costs. The application of perovskite materials in photovoltaic technologies has drawn several scientists and companies. The performance of these devices has not yet been fully tuned, as seen by the variety of topologies, manufacturing techniques, perovskite compositions, and charge selective layers that have been proposed. In a traditional perovskite solar cell, the halogenated compounds function as the active layer. Although these materials have a respectable PCE, their instability and toxicity have been shown to be major drawbacks. Lead-based perovskite solar cells are harmful for the environment, thus numerous alternatives have been employed in their stead, including Ti, Ge, Sn, Sb, and Bi. There are two ways to lessen the toxicity of the solar cell: the first is to substitute lead with an analogous element, and the second is to replace lead with a tin-lead alloyed perovskite $(CH_3NH_3Sn_xPb_{1-x})$.[2,3] As a result, lead-free perovskite materials including those based on Sn and Ge have grown in popularity. However, Sn-based perovskite solar cells still have certain drawbacks, including: (1) Volatile in naturalistic environments; (2) Sn^{2+} is quickly oxidized to Sn^{4+}. As a member of the same family as tin and lead, germanium (Ge)-based