COMPREHENSIVE STUDY OF $FAGeI_3$ LEAD-FREE PEROVSKITE SOLAR CELLS: A SCAPS -1D SIMULATION

A DISSERTATION

SUBMITTED IN PARTIAL FULFILMENT OF THE REQUIREMENTS
FOR THE AWARD OF THE DEGREE
OF

MASTER OF SCIENCE

in

Physics

Submitted by

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(23/MSCPHY/30)

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June 2025

DECLARATION

I hereby certify that the work which is presented in Project Dissertation-II entitled "**COMPREHENSIVE STUDY OF $FAGeI_3$ LEAD-FREE PEROVSKITE SOLAR CELL: A SCAPS -1D SIMULATION**" in fulfillment of the requirements 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, carried out during a period from August 2024 to May 2025, under the supervision of **Dr. Sarita Baghel**.

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Title of the paper: Comprehensive Study of $FAGeI_3$ Lead-free Perovskite Solar Cell: A SCAPS-1D Simulation.

Author names (in sequence as per research paper): Manabendra L. Bhuyan, Vanshika Vanshika, Vishal Deswal, Sarita Baghel

Name of Journal: *Physica status solidi (a)* – applications and materials science (pss a), Wiley-VCH

Status of paper (Accepted/Published/Communicated): revised manuscript submitted, final decision awaited

Date of paper communication: March 6, 2025

Date of paper acceptance: N/A

Date of paper publication: N/A

Manabendra lal Bhuyan

Place: Delhi **Manabendra Lal Bhuyan (23/MSCPHY/30)**

Date: June 8, 2025

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Place: Delhi
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ABSTRACT

The environmental concerns surrounding lead-based perovskite solar cells (PSCs) have prompted the exploration of eco-friendly alternatives. In this study, the potential of germanium-based perovskite, $FAGeI_3$, is evaluated as a non-toxic, lead-free absorber material for PSCs. Utilizing SCAPS-1D simulation software, the device architecture FTO/ZnSe/$FAGeI_3$/V_2O_5 achieved an optimal power conversion efficiency (PCE) of 14.47%. The influence of critical parameters—including the selection of charge transport layers, absorber layer thickness, defect density, electron affinity of the absorber, and operating temperature on device performance was systematically investigated. The results highlight $FAGeI_3$ as a promising candidate for the development of high-efficiency, sustainable perovskite solar cells.

ACKNOWLEDGEMENT

I extend my heartfelt gratitude to **Dr. Sarita Baghel**, whose guidance has been more than academic; it has been anchoring. Her clarity, quiet encouragement, and unwavering support gave direction not only to this research but to the researcher as well. In every stage of this journey, her patience stood like a calm teacher amidst all my uncertainties.

My sincere thanks to the **Department of Applied Physics, Delhi Technological University**, for providing a nurturing environment, access to essential resources, and the support of dedicated faculty and staff. Their collective presence and expertise created the space in which this research could unfold.

Special gratitude goes to the **PhD scholars under my supervisor**, especially for their time, assistance, and patient collaboration. Their quiet dedication behind the scenes made more difference than words can capture and helped me navigate this process far more smoothly than I could have alone.

I owe much gratitude to my classmates and peers, whose conversations helped sharpen my thinking and occasionally soften the weight of the work.

I gratefully acknowledge the developers of **SCAPS-1D**, University of Gent, Belgium, for creating the simulation tool that underpinned this research.

And to all the electrons who longed to return, but were extracted before they could recombine.

Manabendra lal Bhuyan

Manabendra Lal Bhuyan (23/MSCPHY/30)

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LIST OF SYMBOLS

Symbol	Description
J_{SC}	Short Circuit Current
V_{OC}	Open Circuit Voltage
E_g	Bandgap
χ	Electron Affinity
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
N_t	Defect density

LIST OF ABBREVIATIONS

Abbreviations	Description
PSC	Perovskite Solar Cell
FF	Fill Factor
PCE	Power Conversion Efficiency
HTL	Hole Transport Layer
ETL	Electron Transport Layer
SCAPS-1D	Solar Cell Capacitance Simulator 1D
FTO	Fluorine-doped Tin Oxide
DoS	Density of States

CHAPTER 1

Introduction

Energy is a basic need for modern society; without it, our entire way of living would not function. Relying too much on non-renewable sources like fossil fuels harms the environment and is not sustainable in the long run. One important way to deal with the growing energy crisis and the negative effects of non-renewable energy is to increase the use of renewable energy technologies.[1] More than just an alternative, solar energy represents the Earth's most generous and reliable inheritance. Perovskite solar cells (PSCs) are a promising new type of solar technology that uses organometal halide materials to absorb light and can reach high power conversion efficiency (PCE).[2] However, one major issue with PSCs is that best-performing PSCs often contain lead, which is a toxic material and harmful to health and the environment.

1.1 Problem Statement

1.1.1 Global Energy Trends and Challenges

Global energy demand has been rising at an unprecedented pace, driven by rising industrial activity, expanding cities, and the rapid proliferation of digital technologies. In 2024 alone, global energy consumption increased by 2.2%, surpassing the average annual growth rate of 1.3% observed over the previous decade.[3] This surge was primarily due to electricity demand growing by 4.3%, almost twice the average of the last decade.[4] Although significant advancements have been made in renewable energy deployment, fossil fuels dominate as an energy source in meeting global energy needs. In 2024, natural gas demand grew by 2.7%, reaching a new all-time high, while coal demand increased by just over 1%, also hitting a record level.[5] These trends can be seen more in emerging economies, where rapid economic growth drives higher consumption of non-renewable resources. The continued reliance on fossil fuels has led to a rise in energy-related carbon dioxide emissions, which increased by 0.8% in 2024, reaching 37.8 billion tonnes.[3] This

trajectory poses significant challenges to global climate goals, as the emissions from fossil fuel combustion remain a primary contributor to global warming and environmental degradation.

The persistent growth in energy demand, with the continued dependence on non-renewable energy sources, underscores the need for an urgent shift to sustainable energy systems.

1.1.2 Renewable Energy and Perovskite Solar Cells.

The global focus is increasingly shifting toward renewable energy solutions, to counteract this accelerating strain on non-renewable energy sources and the resulting environmental consequences. Among these, solar energy is explored extensively due to its abundance and sustainability. Solar technologies have seen rapid development, and innovations to push efficiency boundaries. PSCs have proven to be a promising solar cell type. Their high power conversion efficiencies, low manufacturing costs, and material flexibility make them strong candidates for next-generation solar energy systems.[2]

Despite their remarkable power conversion efficiencies, lead-based perovskite solar cells in their current form pose a significant environmental and health risk caused by the inherent toxicity of lead. These high-performing, scalable, and low-cost PSCs, raise serious concerns regarding exposure of lead to the environment having harmful long-term effects on ecosystems and human health. This challenge highlights a critical trade-off between performance and sustainability, the development of non-toxic or lead-free alternatives is an urgent priority in advancing PSC technology.

1.2 Objective and Scope

To mitigate the ecological and health hazards linked to lead-containing perovskite solar cells, researchers have increasingly focused on identifying non-toxic alternatives that maintain comparable efficiency and optoelectronic properties. One such promising candidate is germanium (Ge), an element from the same group as lead (Pb), offering similar valence configurations and the potential to form stable perovskite structures.[6] Studies have demonstrated that germanium-based halide perovskites such as those utilizing methylammonium (MA) and formamidinium (FA) as A-site cations, hold

considerable promise in photovoltaic applications.[7] $FAGeI_3$ has been explored experimentally and with other similar materials in DFT-based calculations. DFT-based calculations have demonstrated the promising potential of $FAGeI_3$, revealing its favorable electronic and optical properties.[8,9] Roknuzzaman et al. showed that $FAGeI_3$ exhibits absorption spectra comparable to its lead- and tin-based counterparts ($FAPbI_3$ and $FASnI_3$), demonstrating its potential as a viable lead-free alternative for perovskite solar cell absorbers.[9] However, experimental synthesis of $FAGeI_3$ has yielded mixed results, with initial reports indicating poor film morphology and a measured band gap of approximately 2.35 eV,[10] while subsequent studies achieved better film quality with an experimentally determined band gap closer to 2.2 eV, a value adopted in this work.[7] $FAGeI_3$ has strong absorption in the visible spectrum, making it effective for capturing sunlight.[8] Apart from these calculations and experimental measurements, there has been limited work on this material, reporting the simulation of this material functioning as an absorber layer within the PSC. This forms the basis of the present work, which aims to investigate the applicability of $FAGeI_3$ as a lead-free absorber material through numerical simulations.

1.3 Overview

In this work, a $FAGeI_3$-based perovskite solar cell (PSC) is numerically tuned by adjusting absorber thickness, concentration of defects, electron affinity, and temperature. The Electron (ETL) and Hole transport layer (HTL) must exhibit proper energy level matching with the perovskite layer to facilitate efficient charge extraction and electric field modulation. Beyond electronic roles, the ETL and HTL also enhance device stability by suppressing ion migration, passivating defects, and reducing recombination. They influence optical properties as well, affecting light propagation and spectral response. Given their multifunctionality, this study evaluates alternative ETL and HTL materials through simulation, highlighting their critical impact on overall device performance.

The investigation of $FAGeI_3$, particularly with respect to its temperature-dependent optoelectronic and structural properties, presents new opportunities for realizing PSCs that are efficient, stable, and environmentally benign PSCs.

CHAPTER 2

Literature Review

2.1 Renewable Energy Sources

Since 1970s oil crisis, global interest in renewable energy has grown significantly. In recent decades, renewables have also gained attention for their potential to address critical global challenges spanning technical, environmental, economic, and geopolitical domains.[1]

Renewable energy mirrors the natural cycle; it is an inexhaustible and self-renewing resource. Unlike fossil fuels, these sources are considered sustainable as their replenishment rate is much higher than energy consumption or needs and generally exert lower environmental impacts. The primary types include solar energy, wind energy, hydropower, geothermal energy, and biomass energy.[11]

2.2 Solar Cells

Solar cells generate electricity from sunlight. They generate electrical power by producing both a voltage and a current when exposed to light, based on the photoelectric effect. This process requires two key steps: first, a material must absorb light, which excites an electron to the conduction band. Second, excited electrons must leave the solar cell and flow into an external circuit, leading to a unidirectional current flow. The main types of solar cells include:

- **Crystalline Silicon Solar Cells**: The most common type, known for their high efficiency and durability.[12]
- **Thin-Film Solar Cells**: They are lightweight and flexible solar cells made by depositing one or more thin layers of photovoltaic material onto a substrate.[13]

- **Perovskite Solar Cells**: Emerging technology that has shown rapid efficiency improvements and offers potential for low-cost production.[14]

While silicon-based solar cells continue to lead the market, supported by a mature and well-integrated manufacturing ecosystem, their performance improvements have plateaued. Consequently, PSCs have gained considerable interest in recent years due to their rapid efficiency increase in a short period. Researchers are exploring advanced materials with higher absorption coefficients that can capture more sunlight, to enhance the efficiency of the solar cells.

2.3 Perovskite Solar Cells

PSCs use Perovskite materials as an absorber layer, that absorbs the incident light and generates free charge carriers. Perovskite materials have the structure ABX3 (where A is a monovalent cation like $CH_3NH_3^+$ known as MA^+, $CH(NH_2)^{2+}$ known as FA^+ and Cs^+; B is metal cations like Pb^{2+} and Sn^{2+}; and X for halide ions: I^-, Br^- and Cl^-).[2]

PSCs consist of an HTL, Absorber layer, ETL, and front and back contacts. The Solar device has a structure that is back contact (metals like Ag/Au are used) is connected to the HTL, the absorber layer is sandwiched between HTL and ETL, and the ETL is connected to a front contact like (FTO, ITO, etc) as shown in **figure 2.1**.[15]

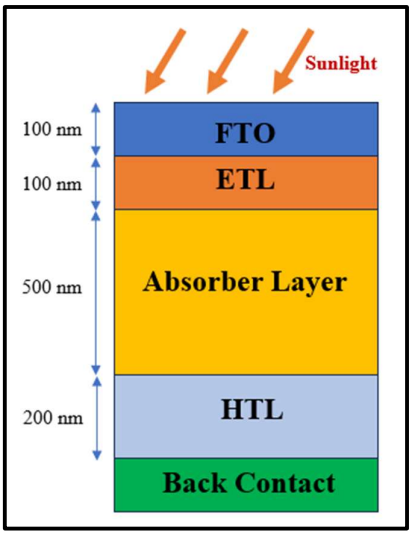


Figure 2.1: Device architecture of Perovskite Solar Cell

From its early development research in PSCs has shown a rapid boost in efficiency in a short period, where the stability remained a major challenge.

Kozima *et al.,* in 2009 introduced $MAPbX_3$ (X- halides) perovskites as light absorbers in dye-sensitized solar cells, achieving 3.8% PCE. However, the use of liquid electrolytes led to rapid degradation of the PSC.[16]

In 2012, a significant breakthrough occurred when Henry Snaith's group replaced the liquid electrolyte with a solid-state HTL (Spiro-OMeTAD), achieving a PCE of 9.7% and enhancing device stability.[17] Over the years significant advancements through were made in PSCs achieving PCE beyond 20% by developing better deposition methods, optimizing the perovskite compostion and device architectures. Later, efforts focused on enhancing stability and scalability. Innovations included the development of tandem solar cells combining perovskite and silicon layers, achieving efficiencies exceeding 25%.[18] Notably, the incorporation of formamidinium lead iodide ($FAPbI_3$) improved thermal stability and bandgap alignment.[19]

In recent years research into lead-free perovskites, such as gemanium-based alternatives, progressed, with promising efficiencies. While offering environmental benefits, challenges remain in achieving comparable stability and performance to lead-based counterparts.[6-10]

2.3.1 $FAGeI_3$-based PSC

In this study, $FAGeI_3$ (formamidinium, $HC(NH_2)_2GeI_3$) is a germanium-based perovskite material being explored as a lead-free alternative to the widely used lead-based perovskite, $FAPbI_3$, in solar cell applications. $FAGeI_3$ addresses environmental and safety concerns associated with lead toxicity. Its potential to support high-efficiency devices without relying on toxic components makes it a promising candidate for next-generation PSCs. However, despite its promise, limited research has been conducted on $FAGeI_3$, as a material and an absorber layer in PSCs. The scarcity of experimental studies highlights its untapped potential and the need for further investigation. The purpose of this research is to contribute to this emerging field by exploring the performance of $FAGeI_3$-based PSCs and assessing their viability as environmentally friendly and stable alternatives to high-performing lead-based counterparts. The detailed device architecture, simulation parameters, and further analysis are discussed in the subsequent sections.

CHAPTER 3

Device Structure and Methodology

3.1 Structure

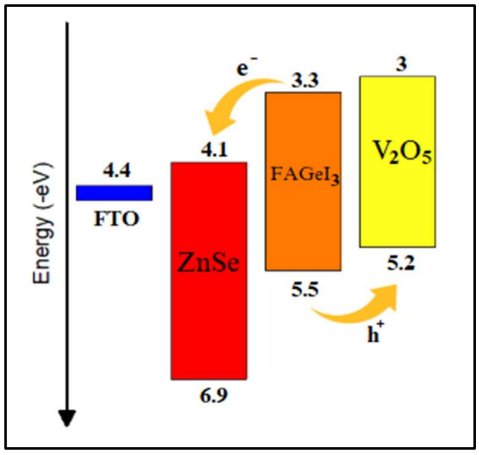


Figure 3.1: Band alignment for $FAGeI_3$-based Perovskite Solar Cell

Various structures of the $FAGeI_3$-based PSC have been formed by employing different ETLs and HTLs. The parameters of the materials used as ETLs, HTLs, FTO, and the absorber layer used are mentioned in **Table 3.1** and **Table 3.2**. The intrinsic parameters have been sourced from previously published studies, while the remaining values are estimated from available experimental and simulation data. The range of parameters of FTO, ETL, and HTLs has been optimized in earlier works. The ETL and HTL pair showing the best performance in the optimization has been selected for subsequent simulations. These simulations focus on the effect of different thicknesses, electron affinity, and the absorber layer's defect density, $FAGeI_3$, on the device functioning. The density of states of the valence band and conduction band of the absorber layer is calculated using the formula.[20]

$$N_{c/v} = 2(\frac{2\pi k_b T m^*_{e/h}}{h^2})^{\frac{3}{2}}$$

where $m^*_{(h/e)}$ is the effective of the hole and electron mass, and,

$N_{c/v}$ is the DoS of conduction and valence bands.

A comparatively low defect density of 1×10^{11} cm^{-3} is used, as high-quality materials with fewer defects help reduce non-radiative recombination, a major cause of energy loss in solar cells.[21]

Table 3.1: Initial input parameters of FTO, $FAGeI_3$, and different ETLs used

Parameters	FTO [20]	$FAGeI_3$ [7,20]	ZnSe [20]	TiO_2 [20]	IGZO [20]
Thickness (nm)	100	500	100	100	100
E_g (eV)	3.5	2.2	2.81	3.2	3.050
X (eV)	4.5	4	4.09	4	4.160
$\varepsilon/\varepsilon_o$	9	7.12	8.6	9	10
N_c (cm^{-3})	2.2×10^{18}	1.34×10^{19}	2.2×10^{18}	2×10^{18}	5×10^{18}
N_v (cm^{-3})	1×10^{19}	1.66×10^{19}	1.8×10^{18}	1×10^{19}	5×10^{18}
μ_h ($cm^2 V^{-1} s^{-1}$)	2×10^{3}	2×10^{-4}	110	10	0.1
μ_e ($cm^2 V^{-1} s^{-1}$)	2×10^{3}	2×10^{-4}	400	20	1.5
V_e ($cm\ s^{-1}$)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
V_h ($cm\ s^{-1}$)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
N_D (cm^{-3})	2×10^{19}	-	1×10^{15}	9×10^{16}	1×10^{17}
N_A (cm^{-3})	-	-	-	-	-
N_t (cm^{-3})	1×10^{15}	1×10^{11}	1×10^{15}	1×10^{15}	1×10^{15}

Table 3.2: Initial input parameters of different HTLs used

Parameters	CBTS [22]	p-$FAGeCl_3$ [23]	V_2O_5 [22]	CFTS [22]	PEDOT: PSS [22]
Thickness (nm)	200	200	200	200	200
E_g (eV)	1.9	3.34	2.2	1.3	1.6
X (eV)	3.6	2.45	4	3.3	3.4
$\varepsilon/\varepsilon_o$	5.4	3	10	9	3
N_c (cm^{-3})	2.2×10^{18}	2.5×10^{18}	9.2×10^{17}	2.2×10^{18}	2.2×10^{18}
N_v (cm^{-3})	1.8×10^{19}	1.8×10^{19}	5×10^{18}	1.8×10^{19}	1.8×10^{19}
μ_h ($cm^2 V^{-1} s^{-1}$)	10	2×10^{-4}	4.0×10^{1}	21.98	4.5
μ_e ($cm^2 V^{-1} s^{-1}$)	30	2×10^{-4}	3.2×10^{2}	21.98	4.5
V_e ($cm\ s^{-1}$)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
V_h ($cm\ s^{-1}$)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
N_D (cm^{-3})	-	-		-	-
N_A (cm^{-3})	1×10^{18}	1×10^{19}	1×10^{18}	1×10^{18}	1×10^{18}
N_t (cm^{-3})	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{15}	1×10^{15}

3.2 Device Design Method

The SCAPS version 3.3.11 is used to construct the PSC device. The SCAPS 1-D software solves the charge carrier continuity equations and the associated Poisson equation to simulate the solar cell performance. Poisson's equation is given by [24]

$$\frac{d}{dx}\left(-\varepsilon(x)\frac{d\psi}{dx}\right) = q[p(x) - n(x) + N_d^+(x) - N_a^-(x)] \quad (3.1)$$

Where $\varepsilon(x)$ is the permittivity of the material at position x.

ψ – Electrostatic potential.

q – Elementary charge (1.602×10^{-19}C).

$p(x)$, n(x) – Hole and Electron concentration at position x.

$N_d^+(x)$, $N_a^-(x)$ – Ionized donor and acceptor concentration at position x.

Hole and Electron continuity equations are given by Equations 2 and 3,[24]

$$\frac{\partial j_n}{\partial x} = q\left(R_n - G + \frac{\partial n}{\partial t}\right) \quad (3.2)$$

$$\frac{\partial j_p}{\partial x} = -q\left(R_p - G + \frac{\partial p}{\partial t}\right) \quad (3.3)$$

Where $j_{n/p}$ – Electron/hole current density.

$R_{n/p}$ – Recombination rate of electrons/holes.

G – Generation rate of electron-hole pairs by light absorption.

$\frac{\partial n}{\partial t}$ – Time-dependent change in electron concentration.

$\frac{\partial p}{\partial t}$ – Time-dependent change in hole concentration.

3.2.1 SCAPS- 1D Software

SCAPS-1D is an open-source Windows-compatible computational model created by the University of Gent in Belgium for modeling photovoltaic devices. The program allows for simulating up to seven layers, not including contact layers. It is used to analyze key performance metrics such as J-V characteristics, alternating current (AC) response, PCE (η), fill factor (FF), and short-circuit current density (J_{sc}), providing a key understanding

of the physical behavior and material properties of PSCs. By simulating perovskite solar cells (PSCs), one can better understand device fundamentals and their response to various external influences. All simulations in this study were conducted under the exposure of Air Mass (AM) 1.5G solar spectrum (temperature at 300 K).

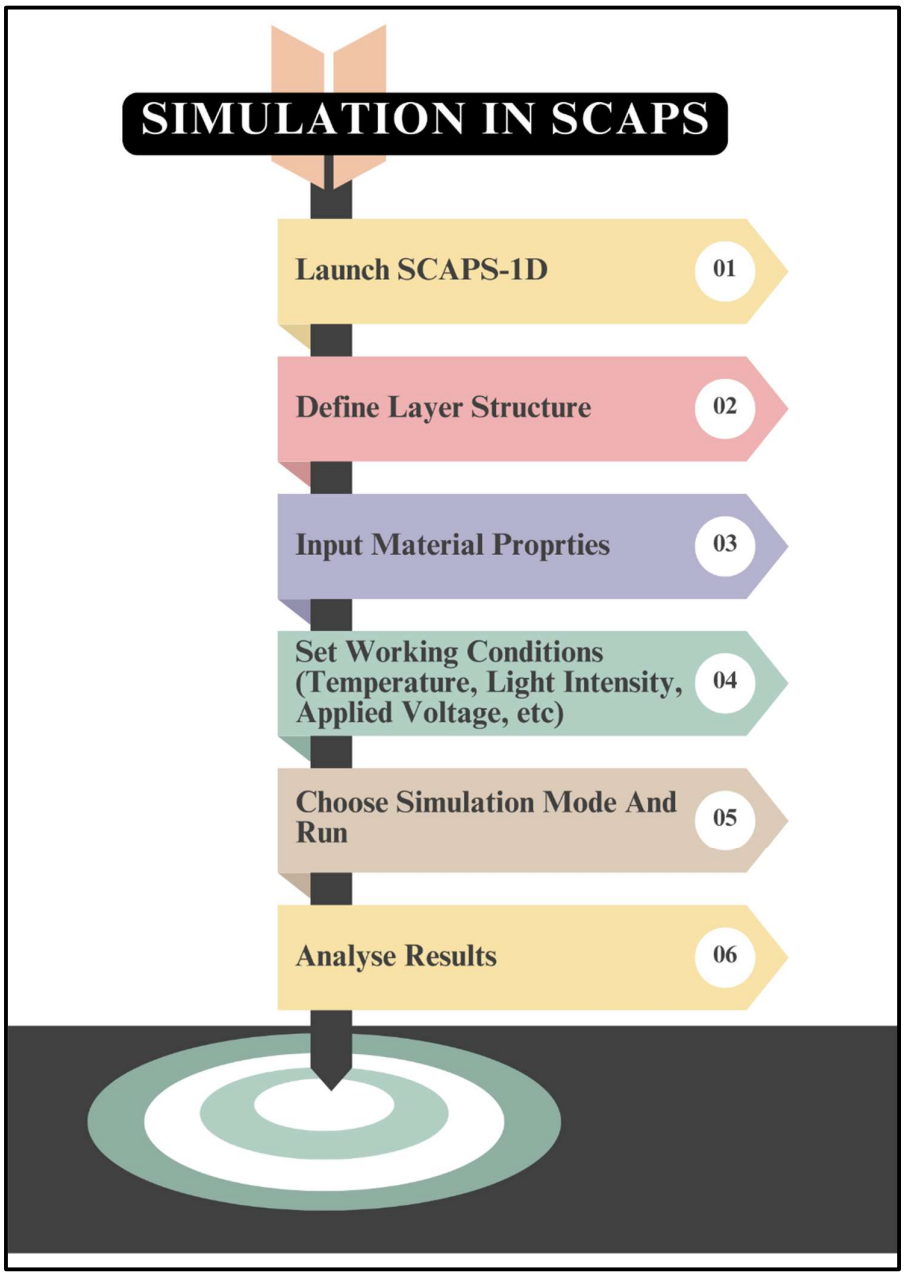


Figure 3.2: Simulation in SCAPS-1D software.

CHAPTER 4

Results and Discussions

4.1 Selection of the Optimized Combination of ETL and HTL

In PSCs, the ETL extracts the photo-generated electrons while bocking holes, preventing them from moving back into the FTO layer. Similarly, the HTL helps transfer holes from the perovskite layer to the anode and stops electrons flowing to the anode. Together, the ETL and HTL keep the charge carriers separated, allowing charge carriers generated in the absorber layer to move in only one direction. Hence, it provides a unidirectional flow of charges leading to the external circuit's current.

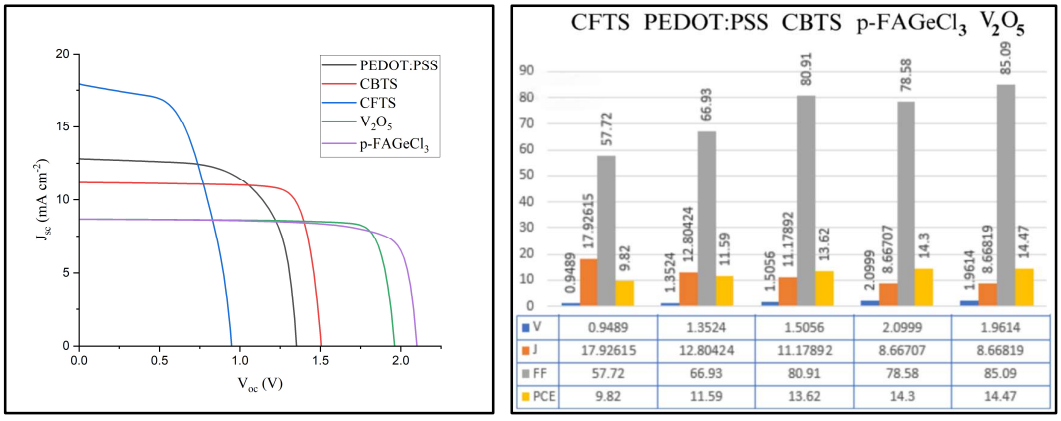
In this study, several ETLs and HTLs have been tested to find the optimal combination that can improve the efficiency of the PSC. Specifically, three ETLs (TiO_2, ZnSe, and IGZO) and five HTLs (CBTS, p-$FAGeCl_3$, V_2O_5, CFTS, and PEDOT: PSS) were chosen because previous research has shown promising results with these materials.[22, 25-29] The alignment of energy bands between these layers and the perovskite absorber is crucial since it affects how well charge carriers can move through the device. [29]

Table 1 and **Table 2** present, the parameters of ETLs and HTLs used in this study for simulation. The simulation results of the device performances of the combinations of various ETLs and HTLs are given in **Table 3**.

Table 4.1: Simulated results for different combinations

SL.	Device Structure	V_{oc} (V)	J_{sc} (mA cm^{-2})	*FF* (%)	*PCE* (%)
01	FTO/IGZO/$FAGeI_3$/CFTS	0.9471	18.471769	53.83	9.42
02	FTO/IGZO/$FAGeI_3$/PEDOT:PSS	1.3509	12.645999	65.82	11.24
03	FTO/IGZO/$FAGeI_3$/CBTS	1.5039	10.963223	79.22	13.06
04	FTO/IGZO/$FAGeI_3$/p-$FAGeCl_3$	2.0981	8.421167	78.02	13.78
05	FTO/IGZO/$FAGeI_3$/V_2O_5	1.9593	8.42206	84.01	13.86
06	FTO/TiO_2/$FAGeI_3$/CFTS	0.9488	19.042345	53.65	9.69
07	FTO/TiO_2/$FAGeI_3$/PEDOT:PSS	1.3523	12.880717	66.06	11.51
08	FTO/TiO_2/$FAGeI_3$/CBTS	1.5052	11.178981	80.61	13.56
09	FTO/TiO_2/$FAGeI_3$/p-$FAGeCl_3$	2.1002	8.633503	78.29	14.2
10	FTO/TiO_2/$FAGeI_3$/V_2O_5	1.9609	8.631515	85.06	14.4
11	FTO/ZnSe/$FAGeI_3$/CFTS	0.9489	17.926147	57.72	9.82
12	FTO/ZnSe/$FAGeI_3$/PEDOT:PSS	1.3524	12.804239	66.93	11.59
13	FTO/ZnSe/$FAGeI_3$/CBTS	1.5056	11.178924	80.91	13.62
14	FTO/ZnSe/$FAGeI_3$/p-$FAGeCl_3$	2.0999	8.667074	78.58	14.3
15	FTO/ZnSe/$FAGeI_3$/V_2O_5	1.9614	8.668185	85.09	14.47

The PSCs using IGZO, TiO_2, and ZnSe as ETL show pretty similar performance overall, but ZnSe comes out on top with the highest efficiency. **Figure 4.1** shows how the device performs with ZnSe as ETL when paired with different HTLs. Among the five HTLs used, CBTS, *p*-$FAGeCl_3$, and V_2O_5 gave better efficiency results. The combination that worked best was FTO/ZnSe/$FAGeI_3$/V_2O_5, reaching an efficiency of 14.47%. Because of this, this particular structure (FTO/ZnSe/$FAGeI_3$/V_2O_5) was chosen for more detailed simulation.



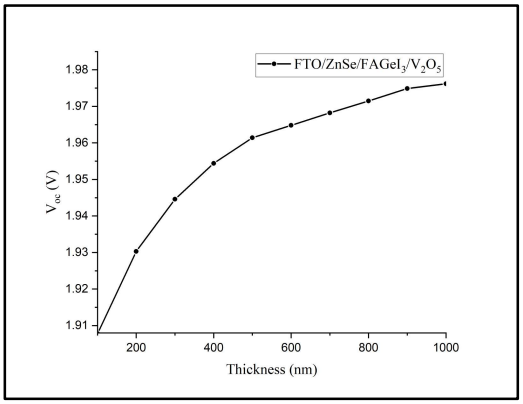
(a) (b)

Figure 4.1: (a) Comparison of J-V characteristics (b) device performance of different HTLs used in the PSC structure with ZnSe as ETL.

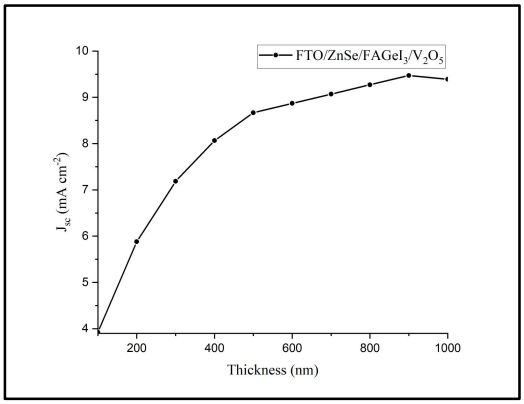
These further studies focused on optimizing the photoactive layer's thickness, defect density, and electron affinity, and observing the temperature effect on the PSC. Band alignment of the PSC layers is shown in **Figure 3.1**.

4.2 Optimization of Thickness of Absorber Layer ($FAGeI_3$)

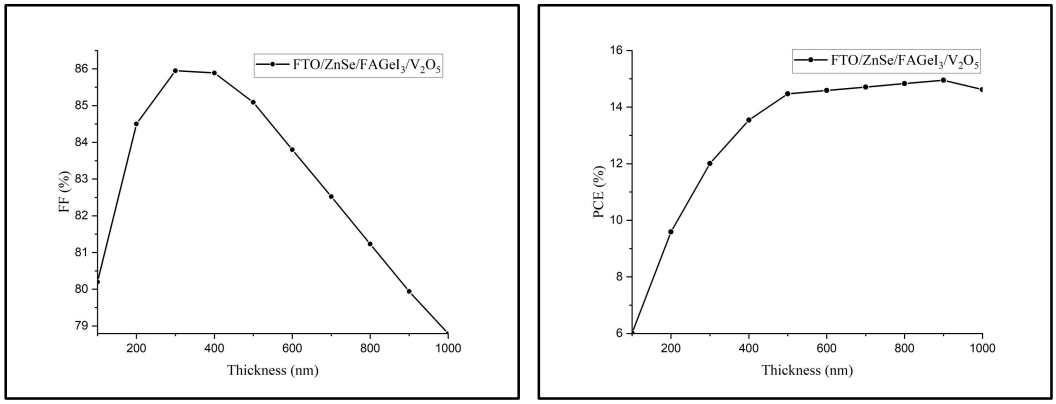
A deep impact on how the PSC performs depends on the absorber layer's thickness. In this work, for device structure FTO/ZnSe/$FAGeI_3$/V_2O_5, the thickness was varied from 100 to 1000 nm, increasing by 100 nm each step. As the absorber layer gets thicker, it can more sunlight is absorbed, which creates more charge carriers, increasing the efficiency. However, if the thickness increases too much, the efficiency drops as the recombination of carriers increases and dominates.[20] The maximum efficiency of the PSC was shown at a thickness of 900 nm, which is 14.95%. Open-circuit voltage increases slightly with increasing thickness, but the J_{sc} rises significantly. The fill factor increases as the thickness increases from 100 nm, attaining a maximum value at a thickness of 300 to 500 nm. The optimized thickness was found to be 500 nm, showing an FF of 85.09% with 14.47% PCE. The thickness of the perovskite layer is used for further simulations.



(a)



(b)



(c) (d)

Figure 4.2: Graph showing the variation of a) V_{oc}, b) J_{sc}, c) FF, and d) PCE to the change in the absorber layer's thickness.

4.3 Optimization of Defect Density

The concentration of defects(N_t) in the perovskite layer significantly impacts device efficiency. When defect levels are high, they cause more recombination of charge carriers, which leads to faster degradation of the film, reduced stability, and poorer overall performance due to issues like pinhole formation [10, 30] For optimization, the defect density was varied from 1×10^7 to 1×10^{14} while keeping the absorber thickness fixed at 500 nm and all other factors constant. As shown in **Figure 4.3**, the PSC performs best at lower defect densities, but efficiency sharply declines as the defect density crosses roughly 10^{12} cm^{-3}, indicating importance of defect management in $FAGeI_3$. This observation is explained by the Shockley-Read-Hall (SRH) recombination:

$$R_{SRH} = \frac{p.n - n_i^2}{\tau_p(n+n_i)+\tau_n(p+n_i)} \quad (4.1)$$

Where R_{SRH} represents the recombination rate. p and n denote hole and electron concentration, whereas their respective lifetime given by τ_n and τ_p. The recombination rate increases with an increase in defect density, reducing the current and overall performance of the PSC.[31]

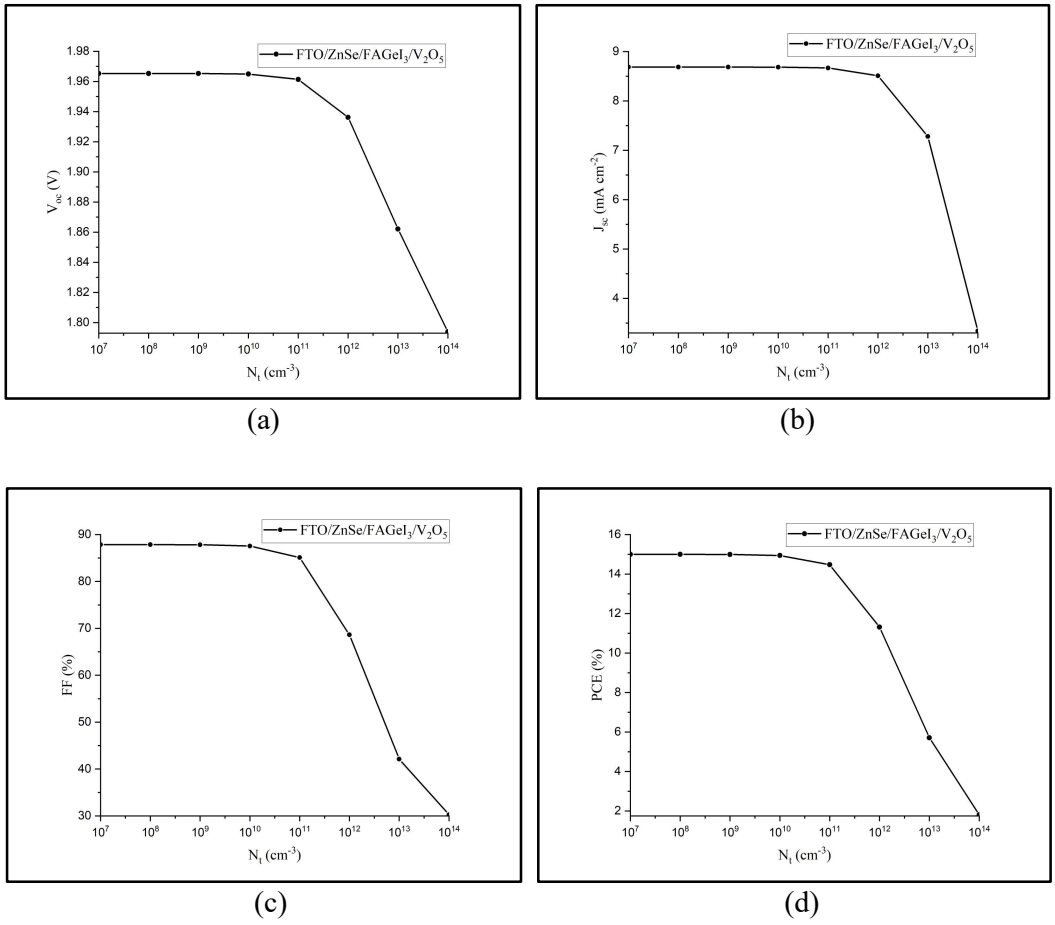


Figure 4.3: Graph showing the variation of a) V_{oc}, b) J_{sc}, c) FF, and d) PCE to the change in the absorber layer's defect density (N_t).

4.4 Tuning of the Electron Affinity of the Perovskite Layer

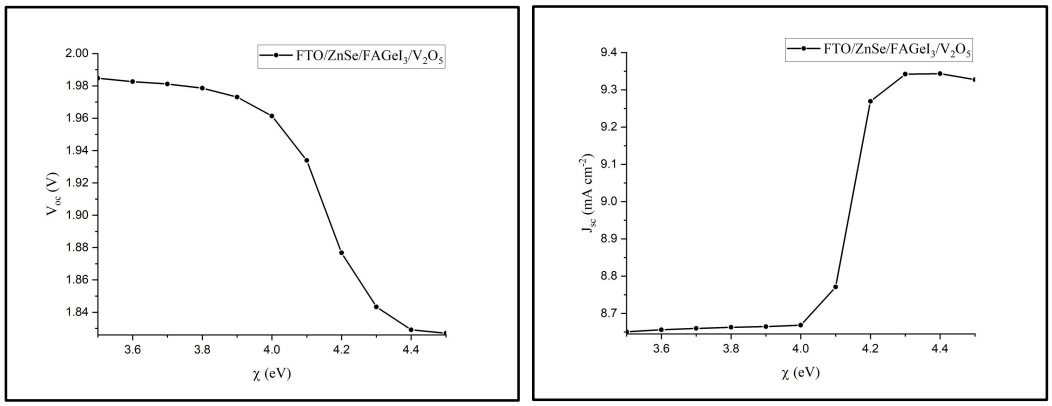
The performance of the PSC also depends on the band alignment of the layers, i.e., CBO and VBO of the various layers of the PSC.[29] Electron affinity (χ) significantly affects CBO and VBO, as described in Equations 5 and 6.

$$CBO = (\chi_{Per} - \chi_{CTL}) \quad (4.2)$$

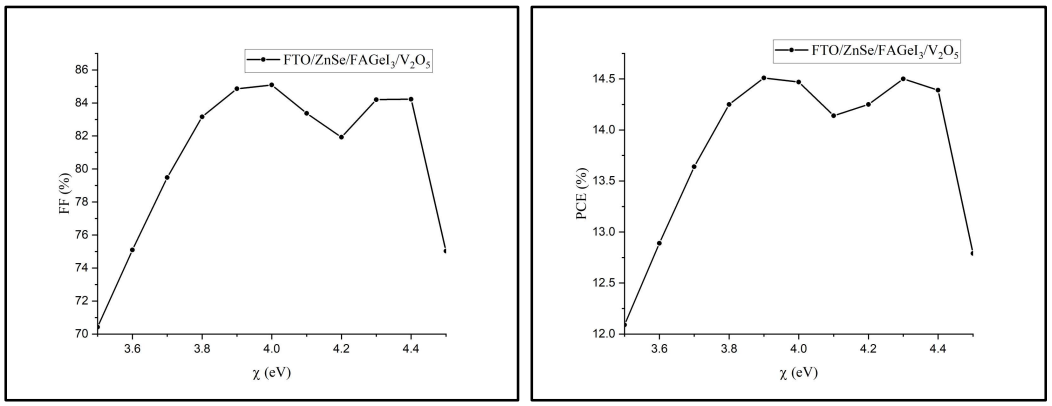
$$VBO = (\chi_{Per} - \chi_{CTL} + E_{g_{CTL}} - E_{g_{Per}}) \quad (4.3)$$

Where, *Per*- Perovskite layer, *CTL*- Charged transport layer, E_g- Band gap energy.

The electron affinity of the absorber layer plays an important role in determining the overall performance of the PSC. [32] The effect of electron affinity is optimized from 3.5 to 4.5 eV while maintaining other parameters the same. This allowed observation of how the cell responds solely to changes in electron affinity. The results show that the PCE improves as the electron affinity increases up to a certain point. The maximum PCE is achieved at values around 3.9 eV and 4.0 eV. The electron affinity value for the simulation is set at 4.0 eV. At this point, the efficiency for the device structure FTO/ZnSe/$FAGeI_3$/V_2O_5 is found to be 14.47%. **Figure 4.4** presents the variation of key performance metrics against electron affinity. The graphs indicate that the efficiency increases initially and then becomes somewhat stable over a narrow range, before starting to decline beyond higher affinity values. V_{oc} shows a decreasing trend after peaking at an electron affinity of 3.5 eV and eventually stabilizes. The FF displays a more noticeable dependence, increasing initially and then dropping again after reaching a peak. Based on this analysis, an electron affinity of 4.0 eV is chosen for the absorber layer, as it maintains a good balance among all performance metrics and results in optimal efficiency for the PSC.



(a) (b)



(c) (d)

Figure 4.4: Graph showing the impact of electron affinity on (a)V_{oc}, (b)J_{sc}, (c)FF, and (d)PCE.

4.5 Effect of Temperature

PSCs, like most optoelectronic devices, are quite sensitive to external environmental conditions, temperature being one of the most crucial. Although earlier studies indicate that the material $FAGeI_3$ remains thermally stable up to around 400 K, its performance characteristics still respond noticeably to changes in temperature. In this study, the device was simulated across a temperature range from 260 K to 460 K to observe how thermal variation influences key parameters. [33] Interestingly, the device performs best at the lower end of this range, around 260 K, where all major parameters including $J_{sc,}$ V_{oc}, FF, and PCE reach their peak values. The result is a gradual decline in device performance, especially in V_{oc} and PCE with increasing temperature, primarily driven by thermal activation of non-radiative recombination pathways.[34] Since solar cells are typically subjected to temperatures above 300 K outdoors, the internal strain and thermal stress within the layered structure increase, disrupting the interfacial contact and promoting structural disarray. **Figure 4.5** illustrates the variations in key performance metrics with temperature.

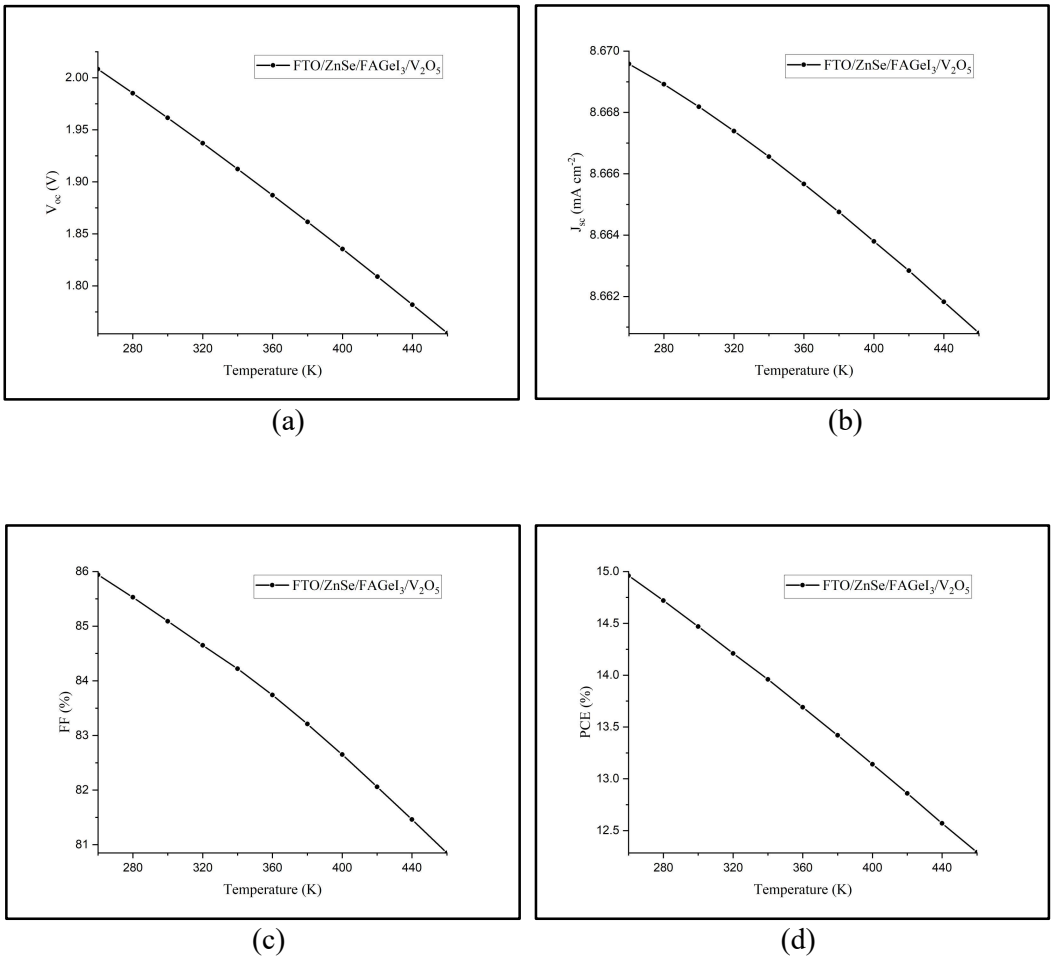


Figure 4.5: Graph showing the variation of a) V_{oc}, b) J_{sc}, c) FF, and d) PCE with Temperature.

4.6 Comparison with Prior Works

Common organic-inorganic perovskite materials such as $MAPbI_3$ and $FAPbI_3$ have long dominated the field of PSCs.[19, 35-37] However, recent investigations into lead-free alternatives have brought germanium-based compounds into the spotlight, with several studies highlighting their potential as viable substitutes for $MAPbI_3$.[15, 38, 39] Despite the growing interest, $FAGeI_3$ remains relatively unexplored as a photovoltaic absorber. While some computational studies particularly those using DFT, have examined its structural,

optical, and electronic properties, practical implementation in the form of a complete solar cell is still lacking.

For instance, Roknuzzaman *et al.* calculated the band gap of $FAGeI_3$ to be 1.04 eV using the GGA-PBE functional and 1.414 eV with HSE06.[9] However, as emphasized by Stoumpos *et al.*, the calculated methods, especially LDA and GGA, are known to underestimate band gaps significantly, and the true optical band gap is likely to be higher.[4] Supporting this, Krishnamoorthy et al. successfully synthesized several Ge-based perovskites including $FAGeI_3$, $MAGeI_3$, and $CsGeI_3$, and tested their photovoltaic responses. While, $CsGeI_3$ and $MAGeI_3$ delivered measurable photocurrent densities, 4 and 5.7 mA cm^{-2}, respectively. $FAGeI_3$ suffered from poor film morphology during synthesis, with a measured band gap of around 2.35 eV, resulting in no observable photocurrent.[7] Another experimental effort reported a slightly lower band gap of 2.2 eV for $FAGeI_3$ and improved material quality, though further progress is clearly needed. [7]

Table 4.2: Performance of the developed solar cell from similar perovskite material.

Device	Reference	J_{sc} (mA cm^{-2})	V_{oc} (V)	*FF* (%)	*PCE* (%)
FTO/ZnSe/$FAGeI_3$/V_2O_5	Simulation [This work]	8.67	1.96	85.09	14.47
FTO/TiO_2/$FAGeI_3$/PTAA	Simulation[40]	15.44	1.26	80.22	15.62
FTO/SnO_2/$MAGeI_3$/$CuAlO_2$	Simulation[15]	16.18	1.77	89.02	25.43
ITO/$PC_{70}BM$/$MAGeI_3$/PEDOT:PSS	Experimental[41]	2.29	0.404	44	0.40
FTO/TiO_2/$CsGeI_3$/Spiro-OMeTAD	Experimental[42]	18.87	0.52	51	4.94
ITO/PEDOT:PSS/$FASnI_3$/C60/BCP	Experimental[43]	23.19	0.84	72	14.5

$MAGeI_3$ demonstrates higher PCE than $FAGeI_3$ (as shown in **Table 4.2**) primarily due to its narrower band gap (1.9 eV), as used in the simulation.[15] This allows a better absorption coefficient for $FAGeI_3$.

While the TiO_2/$FAGeI_3$/PTAA architecture studied by Ali *et al.* exhibits higher PCE, the configuration explored in this work, ZnSe/$FAGeI_3$/V_2O_5 offers several compelling advantages enhancing practical adaptability.[40] Incorporating ZnSe as the ETL improves chemical compatibility with the perovskite absorber and helps reduce non-radiative recombination due to its favorable energy alignment and interfacial properties.[44] Meanwhile, V_2O_5, utilized here as the HTL, is known for its inherent thermal and environmental resilience. It forms a robust, moisture- and oxygen-resistant interface, contributing to the overall device durability. Collectively, using ZnSe and V_2O_5 provides a chemically stable and less reactive environment for $FAGeI_3$, making this device structure a promising candidate for long-term operational stability and suitability for scalable fabrication methods.[45]

CHAPTER 5

Beyond Data: Reflections on Writing a Research Paper

When I started writing the research paper, I thought the difficult part was already over. But it turned out that writing wasn't just about reporting results—it was about making sense of them. As I went through the process, I realized how often writing reveals what we haven't fully understood. Organizing sections, choosing the right words, and deciding what mattered most in the flow of ideas. The simulations gave me values and trends, but writing gave shape to those findings. It helped me see not just what I had done, but how to communicate it clearly. In the end, the paper became more than just a record—it became part of how I understood the work myself.

5.1 The Journey of Writing

The paper went through several stages—none of them quick, and none exactly predictable. At first, I struggled to even begin. I had all the data and graphs, but turning them into a structured argument that made sense took more than I expected. Feedback from my mentors and reviewers helped shape the structure and tone. I rewrote parts, sometimes entire sections, to make the paper clearer. At times it felt tiring, but each round of editing gave me a better grip on what I had done.

A few key things I learned along the way:

- Writing a paper is not about writing perfectly at once—it's about revising again and again.
- Small improvements—better headings, clearer captions, simpler sentences—make a big difference.
- Feedback is not something to fear; it shows what the reader needs that I may have missed.
- Writing helped me grow not just as a student, but as a thinker.

5.2 Reflections on Revisions

After the initial submission, the feedback from reviewers was encouraging; suggesting that the work held value, but also asked for improvements, especially in how the language was presented. The core content remained unchanged, but the way it was said needed refinement. It wasn't about rewriting everything, but about making the same ideas easier to follow and polishing them with better phrasing and structure.

At first, it felt difficult; to see that something as basic as expression could hold back a piece of work. But gradually, it became a quiet learning experience: that clarity matters, that how something is said shapes how it's understood. The revision process reminded me that even small adjustments can bring big improvements and that sometimes the best progress happens not by adding more, but by making things simpler and clearer.

5.3 The Weight and Grace of Waiting

As of writing this chapter, the paper has not yet been accepted. Every morning checking for an email, and every night reminding myself that what's done is done, has taught me that research is not just science. It's also about learning to wait with patience, holding space for outcomes beyond your control. This part of the process—quiet and uncertain—carries its own weight, but also a kind of grace. It teaches steadiness, without needing answers right away.

CHAPTER 6

Conclusion

This study explored the potential of $FAGeI_3$ as a lead-free perovskite absorber material for solar cells using SCAPS-1D simulations. The analysis revealed that device performance is highly sensitive to factors like temperature, absorber thickness, defect density, and electron affinity. Among the simulated architectures, the FTO/ZnSe/$FAGeI_3$/V_2O_5 structure showed the highest efficiency of 14.47% at 300 K. The results suggest that careful engineering and defect management are critical for optimizing the performance of $FAGeI_3$-based devices. While challenges in material synthesis remain, this work highlights $FAGeI_3$'s potential as a promising candidate for stable and environmentally friendly PSCs, encouraging further experimental investigation.

CHAPTER 7

Future Scope

The findings of this study open several promising directions for continued research within the domain of lead-free PSCs, based on $FAGeI_3$ as an absorber. The scope extends beyond the simulated configurations of this study and invites theoretical and experimental advancement.

Future research can focus on refining device architecture by exploring a wider range of ETLs and HTLs to improve energy level alignment and charge extraction. Investigating various back contact metals can further enhance device stability and fabrication compatibility. On the material front, minimizing defect density within the $FAGeI_3$ layer remains essential for reducing recombination losses and boosting efficiency. Additionally, controlled band gap tuning through compositional modifications or strain engineering may enable tailored light absorption, expanding the material's potential in tandem configurations and low-light or indoor photovoltaic applications.

Finally, experimental validation of the simulation results through the synthesis of $FAGeI_3$ material and fabrication of corresponding solar cells will be crucial to assess the real-world applicability of the proposed design. Such studies could bridge the gap between computational predictions and practical implementation, ultimately advancing efficient, stable, and environmentally benign lead-free PSCs.

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APPENDICES

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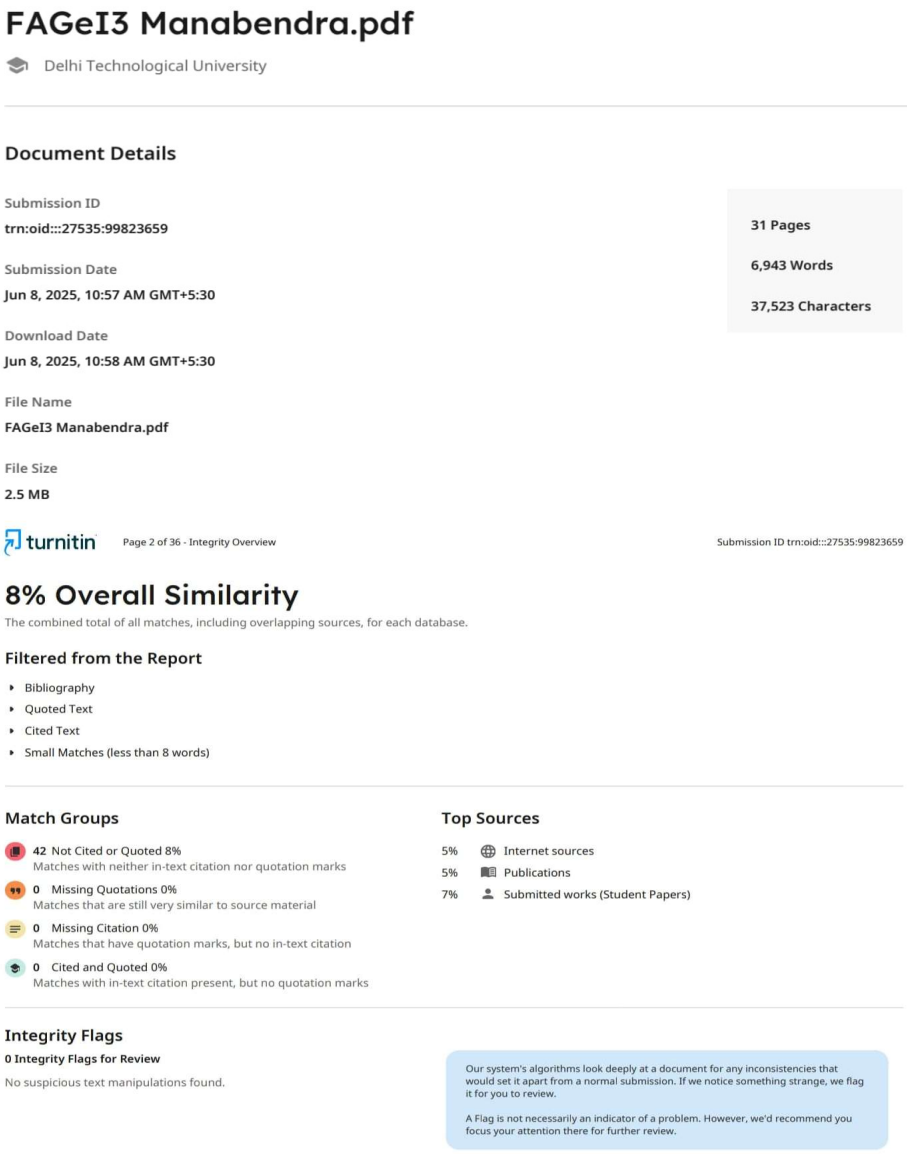

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Dr. Sarita Baghel <saritabaghel@dtu.ac.in> Sun, 25 May, 2025 at 09:29
To: Vanshika Mohan <vanshikam451@gmail.com>, Manabendra Lal Bhuyan <rithee46@gmail.com>

Dr. Sarita Baghel
Assistant Professor
Department of Applied Physics
Delhi Technological University (DTU)
Bawana, Delhi-42

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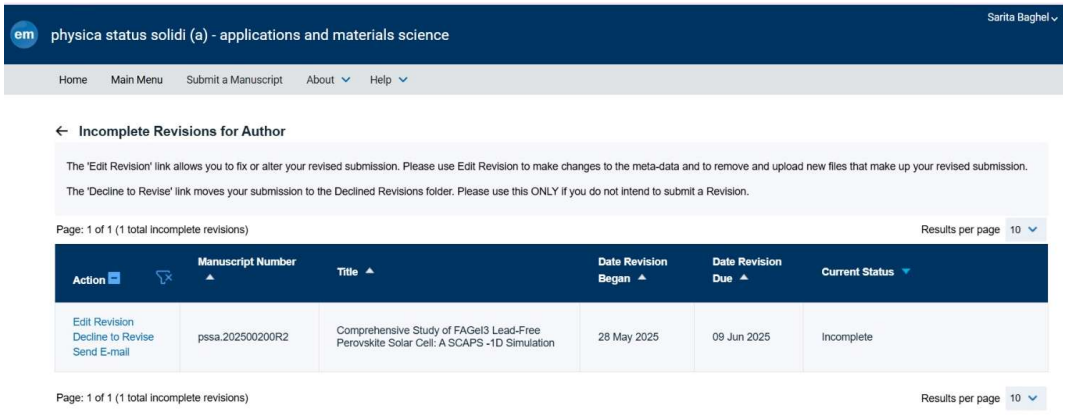

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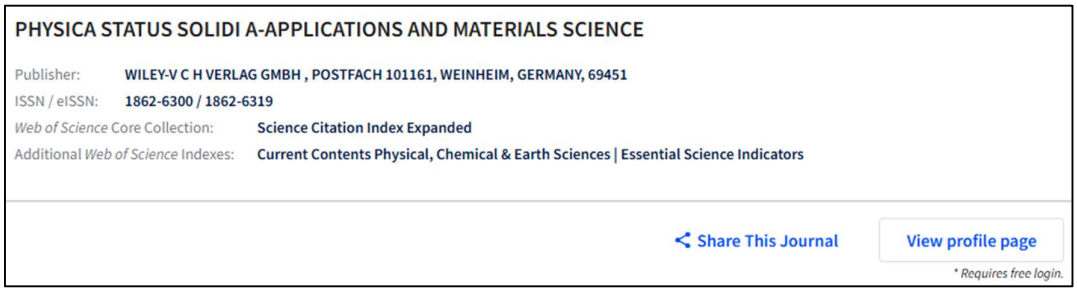

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