SYNTHESIZE OF TIO_2 AS ETL ON FLEXIBLE SUBSTRATE FOR SOLAR CELL APPLICATION

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This report is submitted in partial fulfilment of the requirements for the degree of Bachelor of Electronic Engineering with Honours

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DECLARATION

I declare that this report entitled "**SYNTHESIZE OF TIO2 AS ETL ON FLEXIBLE SUBSTRATE FOR SOLAR CELL APPLICATION**" is the result of my own work except for quotes as cited in the references.

Signature : .....

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Date : 12 JANUARI 2024

APPROVAL

I hereby declare that I have read this thesis and in my opinion this thesis is sufficient in terms of scope and quality for the award of Bachelor of Electronic Engineering with Honours.

Signature : .....

Supervisor Name : TS. MOHD SHAHRIL IZUAN BIN MOHD ZIN

Date : 12 JANUARI 2024

DEDICATION

This thesis is dedicated to my supervisor, Ts. Mohd Shahril Izuan bin Mohd Zin, my co-supervisor, Ts. Dr. Faiz bin Arith, my beloved family members, and my friends.

ABSTRACT

Titanium dioxide (TiO2) possess superior electrical characteristics which is used for perovskite solar cells, that acts as an electron transport layer (ETL). However, TiO2 needs high temperature annealing for crystallization. The purpose of this study is to examine the problems regarding TiO2 as an ETL material in perovskite solar cells and to suggest potential methods to address these concerns. Using TiO2 as an ETL material, the research will comprise a thorough literature analysis of the state-of-the-art in perovskite solar cells with an emphasis on the problems of morphological control, defect development, bandgap restrictions, and environmental considerations. Additionally, experimental work will be done to create and characterize TiO2-based ETLs for perovskite solar cells as part of the project. The management of the synthesis conditions and deposition techniques will optimize the shape of the TiO2 layer. The structural, electrical, and optical characteristics of the TiO2 layer will be examined utilizing a variety of characterization techniques to assess its quality. The study will suggest possible ways to get over the problems of using TiO2 as an ETL material in perovskite solar cells.

ABSTRAK

Titanium dioksida (TiO2) mempunyai ciri-ciri elektrik unggul yang digunakan untuk sel suria perovskit, yang bertindak sebagai lapisan pengangkutan elektron (ETL). Walau bagaimanapun, TiO2 memerlukan penyepuhlindapan suhu tinggi untuk penghabluran. Tujuan kajian ini adalah untuk mengkaji masalah mengenai TiO2 sebagai bahan ETL dalam sel suria perovskit dan mencadangkan kaedah yang berpotensi untuk menangani kebimbangan ini. Menggunakan TiO2 sebagai bahan ETL, penyelidikan ini akan terdiri daripada analisis kesusasteraan menyeluruh mengenai state-of-the-art dalam sel suria perovskite dengan penekanan kepada masalah kawalan morfologi, pembangunan kecacatan, sekatan bandgap, dan pertimbangan alam sekitar. Di samping itu, kerja eksperimen akan dilakukan untuk mencipta dan mencirikan ETL berasaskan TiO2 untuk sel solar perovskite sebagai sebahagian daripada projek. Pengurusan keadaan sintesis dan teknik pemendapan akan mengoptimumkan bentuk lapisan TiO2. Ciri-ciri struktur, elektrik, dan optik lapisan TiO2 akan diperiksa menggunakan pelbagai teknik pencirian untuk menilai kualitinya. Kajian ini akan mencadangkan cara yang mungkin untuk mengatasi masalah menggunakan TiO2 sebagai bahan ETL dalam sel suria perovskite.

ACKNOWLEDGEMENTS

All praises to Allah and His blessings for the completion of this thesis. Throughout my journey to complete this thesis, there were a lot of obstacles that I had to go through. Therefore, I would like to thank Allah for providing me with the strength to go through my PSM journey. The struggle and effort during the process has given me a lot of precious and meaningful memories that I will never forget.

First and foremost, I would like to thank my supervisor, Ts. Mohd Shahril Izuan bin Mohd Zin and my co-supervisor, Ts. Dr. Faiz bin Arith for the guidance, encouragement, and patience from the beginning of PSM 1 until the completion of PSM 2. Both supervisors have been thoughtful and helpful in the context of sharing the knowledge that they have. With that, I thank both for guiding me until the end of the thesis. It has been such a great pleasure and honor to have both of my supervisor, and co-supervisor, respectively.

Finally, I want to extend my sincere thank you to my beloved family for being my main support system. They have been such a help in various forms of emotional support that I really needed.

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LIST OF SYMBOLS AND ABBREVIATIONS

PSC	:	Perovskite Solar Cells
ETL	:	Electron Transport Layer
HTL	:	Hole Transport Layer
TiO_2	:	Titanium Dioxide
HTM	:	Hole-Transporting Material
ETM	:	Electron-Transporting Material
J_{SC}	:	Short-Circuit Current Density
FF	:	Fill-Factor
VOC	:	Open-Circuit Voltage
$CH_3NH_3SnI_3$	:	Methylammonium tin iodide
$CH_3NH_3PbI_3$	:	Methylammonium lead iodide
CuI	:	Copper(I) Iodide

CHAPTER 1

INTRODUCTION (HEADING 1, H1)

1.1 Project Background

As the world's population flourished, day by day, so did the global energy consumption. Environmental problems brought on by the decline in non-renewable energy sources like fossil fuels drive up the use of renewable energy. Due to its abundance, cleanliness, and inexhaustibility, solar energy is regarded as an important renewable energy source in this context. Additionally, using solar energy will not harm the environment [1]. Perovskite solar cells (PSCs) are gaining popularity as a promising photovoltaic technology due to their high efficiency and affordable manufacturing costs. The research on lowering lead leakage and creating environmentally acceptable lead-free perovskites is moving the commercialization of PSCs ahead step by step, and both the efficiency and stability of PSCs have gradually grown in recent years[2]. A solar cell, commonly referred to as a photovoltaic cell or

PV cell, is a type of electrical device that uses the photovoltaic effect to transform light energy into electrical energy. A p-n junction diode is essentially what a solar cell is. A photoelectric cell is a type of device whose electrical properties, such as current, voltage, or resistance, change when exposed to light. Solar cells fall under this category.

A class of materials known as perovskites has a common structural makeup and exhibits a wide range of fascinating features, including superconductivity and magnetoresistance. The unique structure of these readily synthesized materials makes them ideal for permitting affordable, effective photovoltaics, and they are regarded as the solar cell of the future. The batteries, sensors, lasers, and many other components of future electric vehicles are also expected to use them.

A perovskite solar cell is a particular kind of solar cell that uses an organic-inorganic hybrid material based on lead or tin halide as the light-harvesting active layer. Methylammonium lead halides, for example, are inexpensive and reasonably easy to make into perovskite materials. Perovskites are particularly attractive materials for solid-state solar cells because of their inherent features, which include a broad absorption spectrum, quick charge separation, long transport distances for electrons and holes, long carrier separation lifetime, and more.

1.2 Problem Statement

Despite the many advantages of using titanium dioxide (TiO_2) as the electron transport layer (ETL) for perovskite solar cells, there are still several issues that need to be addressed. One of the major problems is the poor interfacial contact between the TiO_2 ETL and the perovskite layer, which can lead to energy loss and reduced

efficiency. This poor interfacial contact can also result in stability issues, such as degradation and hysteresis. In addition, the use of TiO_2 ETLs in perovskite solar cells requires high-temperature processing, which can limit the range of substrates that can be used and increase the manufacturing cost. Therefore, there is a need to improve the interfacial contact between the TiO_2 ETL and the perovskite layer, as well as to develop alternative ETL materials that can overcome these limitations and improve the performance and stability of perovskite solar cells.

1.3 Objectives

1. To design TiO_2 based PSCs using SCAPS-1d software.
2. To analyze several key parameters such as operating temperature, thickness, doping & defect density that effects the power conversion efficiency (PCE) of PSCs.

1.4 Scope of the Project

A research project's scope of work normally involves several crucial activities connected to performing an exhaustive study and compiling pertinent data. Background research, a literature review, and information gathering are the main elements of this scope of work. First and foremost, the background study entails knowing the environment and context of the research subject. It involves learning about the subject, its background, associated theories or concepts, and any pertinent existing data or prior study. This process ensures a thorough comprehension of the topic area and helps lay the groundwork for the research. Multiple important activities relating to the creation and optimization of solar cells utilizing perovskite materials are included in the scope of study for creating perovskite solar cells (PSC) using SCAPS. It is essential to have a thorough understanding of perovskite solar cells

before beginning the design process. Perovskite materials' concepts, traits, and behavior in photovoltaic applications are among the topics covered in this report. This step assists in obtaining understanding of the underlying ideas that guide the creation and operation of PSCs. The next crucial step would be to get familiarized with SCAPS. A popular piece of software for designing and simulating solar cells, particularly perovskite solar cells, is SCAPS (Solar Cell Capacitance Simulator). Understanding how to utilize SCAPS software for PSC design efficiently entails becoming familiar with it, comprehending how it works, and developing the requisite abilities. Designing the perovskite solar cell's structure is the challenge at hand. The layer stack, which includes the transparent conductive oxide (TCO) layer, the perovskite layer, the electron and hole transport layers, and any additional required layers, must be determined. To improve the performance of the device, the design process may also involve optimizing the thickness and makeup of each layer. Not only that, the PSC design can be optimized and simulated using the SCAPS program. To maximize the effectiveness and stability of the device, different parameters, including layer thicknesses, dopant concentrations, and interface qualities, are adjusted. The outcomes of simulations can be examined and used to direct additional design iterations. This is also known as “analysis and data recording”. Overall, the tasks involved in designing perovskite solar cells using SCAPS include learning the basics of PSCs, becoming comfortable with the SCAPS program, designing the PSC structure, choosing appropriate materials, optimizing the design through simulation, assessing performance, and documenting the entire procedure.

1.5 Outline of the Report

The outline of this project report is divided into five chapters: introduction, methodology result and discussion, background study, and conclusion. The idea of using TiO_2 as an ETL layer in evolving solar cells is presented in the first chapter. The goals, description of the problem, and scope of the investigation are then more thoroughly explained. The thesis outline brings this chapter to a close.

The literature is reviewed, and an overview of the developing solar cell is given in the second chapter. This includes the PSC, the fundamentals of P-N semiconductor technology, and previous PSC studies conducted by different researchers.

Chapter 3 introduces the fabrication and simulation techniques. It covered the hardware and software used in considerable detail. The experimental results for TiO_2 simulation are provided in Chapter 4. The corresponding image, graph, and table serve as representations for the technique.

Chapter 5 concludes by emphasizing a comprehensive explanation of the study and simulation. This report also included recommendations for additional work.

CHAPTER 2

BACKGROUND STUDY

This chapter will discuss about sources or articles that related to the project. There are many sources or researchers done before and from there details about this project are known and can understand briefly about the project. In this chapter, the theoretical background, literature reviews of previous work, and the summaries about the previous work will be covered.

2.1 Overview of PSCs

Due to their consistently rising power conversion efficiencies (PCEs) made possible by the intrinsically superior photoelectric qualities of metallic halide perovskites, such as their long carrier diffusion length, robust defect tolerance [3], adjustable band gap (1.0 eV to 3.1 eV), and highlight extinction coefficient (105 cm^{-1}), perovskite solar cells (PSCs) have garnered significant attention from the academic

and industrial communities since 2012. The components of a typical PSC include a metal back contact acting as the anode, a conductive substrate acting as the cathode, an electron transport layer (ETL), a photoactive layer (perovskite), a hole transport layer (HTL), and a photoactive layer sandwiched between the HTL and the ETL. For gathering electrons and obstructing holes, transparent conducting oxides (TCOs) like indium tin oxide (ITO) and fluorine-doped tin oxide (FTO) are the most desirable ETLs. PSCs have achieved the highest power conversion efficiency (PCE) of 25.5%, matching crystalline-Si solar cells in that regard. A perovskite absorber layer and two charge transport layers—typically constructed of spiro-OMeTAD and titanium dioxide (TiO_2) compose PSCs [4]. Considering the numerous benefits, there are still a few problems that need to be resolved when employing TiO_2 as the electron transport layer (ETL) for PSCs. A significant issue is the inadequate interfacial contact between the perovskite layer and the TiO_2 ETL, which can result in decreased efficiency and energy loss.

2.2 Photovoltaic Cell

The most widely used renewable energy source worldwide is solar energy. This is because of its low cost, simplicity of use, clean energy, free energy, and absence of hazardous gas emissions. By using this source, one may lessen reliance on conventional energy sources and fulfil the growing need for electricity. Technologies for producing electricity from solar energy are needed for photovoltaic cells [5]. Since the Sun is expected to last for another 5000–10,000 billion years, solar energy, which is produced from solar radiation, is deemed as renewable. Moreover, this kind of energy is accessible in most of the planet's areas. The photovoltaic effect, which was identified in 1839 by French scientist Alexandre-Edmond Becquerel, allows for the direct generation of electric energy from solar light [6]. This energy is known as

photovoltaic energy (PV). One of the greenest methods of supplying electricity to the globe could be using solar cells. Moreover, most of the environmental impact that is attributed comes from the energy needed for the manufacture and installation of solar panels; this impact is assigned because the present energy technologies have poor environmental qualities. Currently, typical silicon modules installed in generally sunny places have an energy payback period of less than a year, meanwhile thin-film modules are expected to have much shorter payback times [7].

2.3 Characterization of PSCs

The paper by Suleiman Bello et al. (2022) focuses on perovskite solar cells, a field of renewable energy research that is quite active. It goes over hybrid perovskite photovoltaics' operating principles and contrasts them with those of other photovoltaic systems. In the abstract, it is mentioned regarding perovskite material features, production methods, and degradation mechanisms, as well as the present obstacles to the commercialization of perovskite solar cells. This paper attempts to provide a guide for those who are new to the research of perovskite solar cells. Moving onto the introduction, the writer emphasises the significance of producing electricity in a sustainable manner and the requirement for other methods of doing so that are safe for the environment and people's health. It discusses the traditional electric energy source, fossil fuels, and the harmful emissions from these sources of energy that have prompted scientists to look for alternate ways to produce electricity. The introduction also emphasises how renewable energy technologies are evolving, including hydroelectric, wind, solar (thermal and photovoltaic), tidal, and wave power, which are becoming in-trend.

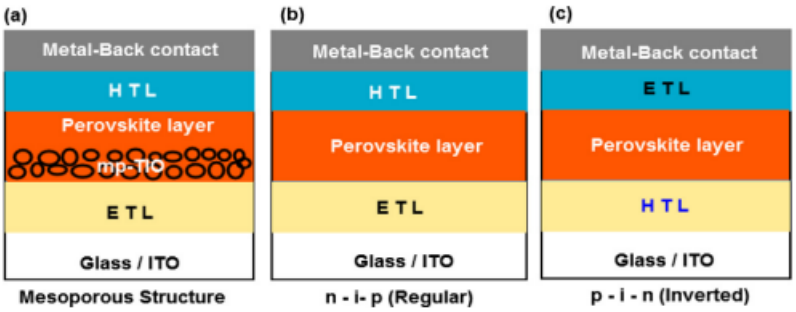

Figure 2.1: Image of schematic illustrations for Perovskite Device Architecture [8]

These devices are constructed from a complete inorganic material, usually consisting of triple cation semiconductors that absorb the incident solar energy, or from hybrid organic-inorganic semiconducting materials. These devices' traditional single-junction construction is comparable to that of bilayer heterojunction organic photovoltaics. Perovskite PVs function differently from organic PVs in terms of their physical process[8].

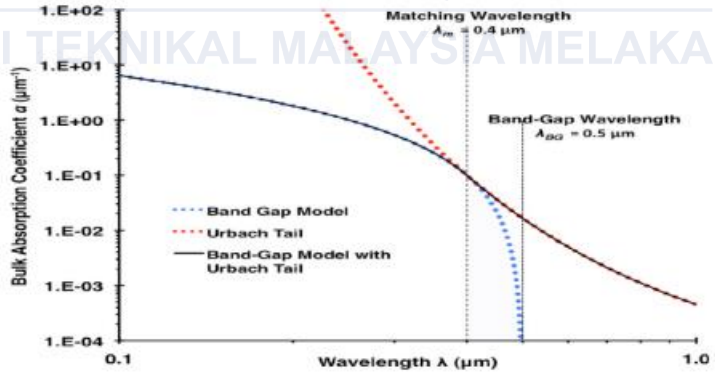

Figure 2.2: Graphical illustration of Urbach-tail and bandgap determination of a semiconductor from UV–Vis absorbance [8]

The author particularly addresses the use of X-ray analysis to provide details about the crystalline structure and characteristics of perovskite in relation to the

characterization of perovskite solar cells. This method can be used to investigate the perovskite's crystalline structure, crystallisation process, and potential existence of harmful unreacted species (such PbI_2). The quality of perovskite thin film can be inferred from the relative intensity between signals (002) and (110), which arise when $CH_3NH_3PbI_3$ separates into two signals during the transition from α cubic phase to β tetragonal phase at 54 ◦C to 60 ◦C. Regardless of the perovskite growth method, the (110) orientation appears to be linked to stronger stability and higher crystallinity than (002).

2.4 Emergence, Progress and Commercialization of PSC

The review paper by Pengyu Zhan et al. (2022) centres on the development of Perovskite Solar Cells (PSCs) as a low-cost, efficient, next-generation photovoltaic technology. It provides a quick overview of PSC development, including everything from discovery to lab research to commercialization. The paper emphasises the huge research efforts on compositional, process, and interfacial engineering that have led to the great achievement in device efficiency and stability over the past several decades, as well as the quick increase in light-to-electric conversion efficiencies of PSCs. The synthesis of narrow bandgap perovskites for solar cell applications and the possibility of PSCs for large-scale roll-to-roll manufacture are also covered in this work. The author explains the extensive research being done since 2009 to increase the efficiency of PSCs, or perovskite solar cells. To improve PSC performance, compositional, process, and interfacial engineering have been the main topics of research. According to the paper, PSCs are ionic compounds whose crystallographic structure may be inferred using the octahedral and Goldschmidt tolerance factors [9]. A chart illustrating the advancement of cell efficiency in perovskite solar cells, single crystal and multi-crystalline ‘Si’ cells, and perovskite/Si tandem is also included in the study.

This chart is based on the National Renewable Energy Laboratory's (NREL) Best Research-Cell Efficiency chart.

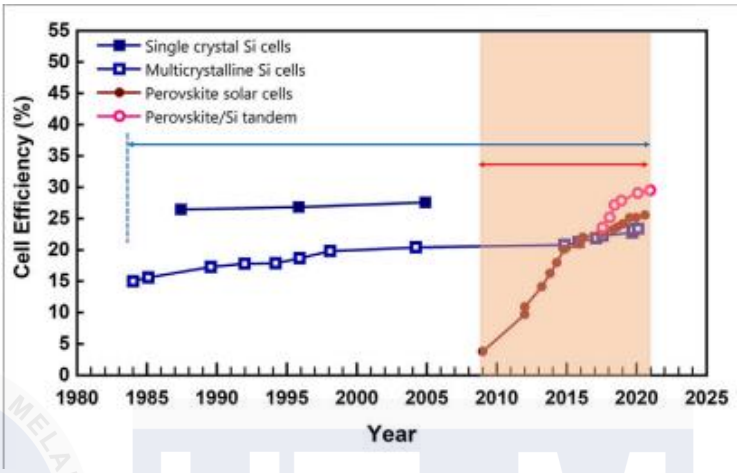

Figure 2.3: Progress of cell efficiency in single crystal and multi-crystalline [9]

2.5 Lead Free PSCs

Lead-free perovskite solar cells have immense potential in mitigating the environmental issues and toxicity that arise from lead-based perovskites. Lead toxicity prevents lead halide perovskites from being produced on a significant scale for commercial use in solar fields. Lead is a substance that is hazardous, polluting, and bio-accumulative that can cause serious harm towards the environment and human health. Therefore, there is the opportunity to enhance the detrimental impacts and sustainability of solar cell technology through the development of lead-free perovskite materials. Since lead-free perovskites may avoid high levels of hazardous risks and are better suited for commercial manufacture and use, they provide an environmentally benign substitute [4]. To create an environmentally benign lead-free perovskite solar cells, a range of non-or low-toxic perovskite compounds have been investigated and it can be said that some of these materials exhibit good optoelectronic properties and

device performances. Perovskites based on tin, bismuth, and double perovskites are a few examples of these materials.

Additionally, there is a chance to enhance the stability and performance of perovskite solar cells through the creation of lead-free perovskite materials, which could result in advances in efficiency and commercial viability. Significant progress has been made in the experimental research of lead-free perovskites, including the determination of the crystal structure and material bandgap for all lead-free materials as well as the stability and photovoltaic performance of matching devices [4]. The successful development and commercialization of lead-free perovskite solar cells still face certain obstacles, nevertheless, such as the requirement for additional lead-free perovskite materials with adjustable optical and electrical characteristics.

The paper by Asir Eliet Magdalin et al. (2023) describes the spotlight on lead-free perovskite solar cells and highlights on how they can be used as sustainable and ecologically acceptable substitutes for conventional lead-based perovskite solar cells. The authors emphasized how lead's toxicity and the ensuing health and environmental issues have impeded the commercialization of lead-based perovskite solar cells. This emphasizes the need for non-toxic, long-lasting substitutes, which prompts research into lead-free perovskite solar cells as a possible remedy.

An overview of the possibilities of different alternative metals in lead-free perovskite solar cells, including tin, germanium, titanium, silver, bismuth, and copper, is given in the introduction.

Figure 2.4: Toxicity of lead in humans [10]

The figure above shows how harmful lead is to people. The graphic illustrates the three main ways that lead, a hazardous heavy metal, may enter the human body through the gastrointestinal tract, the skin, and the lungs [10]. Lead enters the body through the mouth and travels to the liver, kidney, brain tissue, and bones, among other soft tissues. These tissues serve as the body's repository for lead. This may interfere with hem activity in the blood as well as the action of enzymes and receptors in soft tissues.

The effects of lead on the reproductive systems of men and women are also depicted in the illustration. Lead poisoning can result in miscarriages and early births in

females, but it can also lower the sperm count in males. The graphic draws attention to the detrimental impact that lead-substances has on both the environment and human health, emphasizing the need for non-toxic, sustainable alternatives like lead-free perovskite solar cells.

The paper by Shuaibu Sani et al. pivots on the study of defect, doping and the performance of various ETLs. Amongst the ETLs that are sampled in this study are ZnO, TiO_2, and IGZO to be implemented on lead-free $CsSnCl_3$ PSCs. Starting off in the abstract, the authors highlighted the potential of lead-free perovskite materials by using cesium as an organic cation. The importance of defect engineering was also focused on in the effort of enhancing device performance and long-term stability. The acquired parameters or evaluation was done by using SCAPS. The impact of absorber defects on different ETLs is investigated in this work, which emphasizes the effect of defect density on device performance.

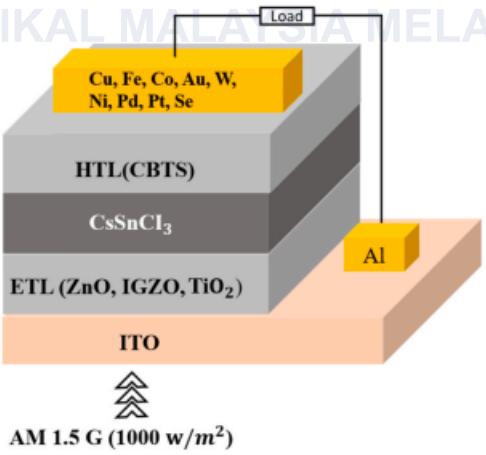

Figure 2.5: Schematic diagram of the proposed perovskite device [11]

The figure above shows the schematic diagram of the proposed perovskite device. It illustrates the layers that are used to make-up the overall PSC. The substrate is typically made of glass or plastic and it can provide a stable base for the device. The

ETL which is varied, is said to facilitate the movement of electrons from the perovskite absorber layer to the electrode layer. Moreover, the perovskite absorber layer, which is $CsSnCl_3$ in the study, acts as the active layer of the device. This means, it acts as a terminal where light is absorbed and is then converted to electrical energy. The transit of holes from the perovskite absorber layer to the electrode is facilitated by the HTL, which is commonly composed of materials like Spiro-OMeTAD. The top electrode completes the circuit by gathering the electrical energy produced and is usually composed of elements like gold or silver.

The impact of interfacial defects between ZnO, IGZO, and TiO2 electron transport layers (ETLs) and perovskite were examined in this study. The findings suggested that in perovskite solar cell systems, interfacial imperfections function as trap-assisted interfacial recombination centres. In accordance with the size of the interfacial flaws, the devices with the various ETLs behaved differently. ZnO and TiO2 shown a greater resistance to interfacial imperfections as evidenced by their reduced V_{OC} deterioration in comparison to IGZO [11]. Additionally, the research found that behaviour stayed consistent as the device got closer to 10^{20} cm^{-2} and that variations in the performance parameters were first noticed at interfacial defects larger than 10^{10} cm^{-2}.

2.6 Effect of ETL thickness

The paper by T.M Mukametkali et al. (2023) highlights the importance of the importance of optimizing the thickness of the electron transport layer in perovskite solar cells to improve the overall performance. In the abstract, the authors focus on the use of various techniques such as impedance spectroscopy, photoluminescence, and four-probe conductivity measurements to analyze the effects of TiO_2 thickness on charge transfer and recombination in PSCs.

The investigation of the effect of TiO_2 electron transport layer thickness on charge transfer processes in perovskite solar cells is carried out through a mix of sample preparation procedures and analytical techniques. Perovskite solar cells are manufactured on glass substrates coated with a Fluoride Tin Oxide (FTO) layer during the sample preparation and deposition process. TiO_2 layers are then deposited from TiO_2 sol-gel solution using spin-coating techniques. The analysis methods also require the application of a variety of analytical tools and procedures. These include the four-point probe method for measuring the conductivity of TiO_2 films, thermal deposition for sample preparation, absorption spectroscopy for measuring absorption spectra, pulsed spectrofluorometric for photoluminescence decay kinetics, and impedance spectroscopy for examining charge transfer processes in perovskite solar cells. Atomic force microscopy (AFM) is used for surface topography and thickness analysis.

The study finds that variations in spin-coating rate led to two competitive impacts on the TiO_2 resistance. Impedance spectroscopy shows that the resistance of TiO_2 decreases with thickness reduction from 120 nm to 90 nm, reaching a minimum at 60 nm, even though an increase in spin-coating rate causes a reduction in TiO_2 thickness and the anticipated decrease in resistance [12]. However, additional thickness reduction results in a rise in TiO_2 film resistance, suggesting that thickness and resistance have a complicated connection. In terms of the charge transport mechanism, the authors show that electron transport via the TiO_2 conduction band and electron trapping by deep trap levels created by Ti^{+3} species are the two competitive charge transport mechanisms that take place in the TiO_2 electron transport layer (ETL). Under the deposition conditions, the balance between both processes is determined to be best at a TiO_2 thickness of about 60 nm, improving perovskite solar cells' performance.

2.7 Metal-Doped TiO_2 Thin Film as an Electron Transfer Layer for Perovskite Solar Cells

The paper by Dewi Suriyani Che Halin et al. (2023) primarily targets on the use of metal-doped TiO_2 thin film as an ETL for PSCs. It contains a thorough analysis of the traits, problems, and disadvantages of TiO_2 ETLs and addresses how to use various metal-doping materials to enhance the doped TiO_2 ETL's bulk properties.

The features of the electron transfer layer (ETL) in perovskite solar cells are covered in detail in this review paper. Given that it makes it easier for electrons to be efficiently collected and transported between the perovskite layer and the electrodes, the ETL is essential to the operation of perovskite solar cells. The study highlights several crucial ETL features that are necessary to maximize solar cell performance. First, the ETL's energy level alignment is emphasized as a critical component. The short-circuit current density (J_{SC}) and fill factor (FF) will rise when the energy level of the ETL and the perovskite layer are matched. This is because it speeds up electron extraction and transport qualities.

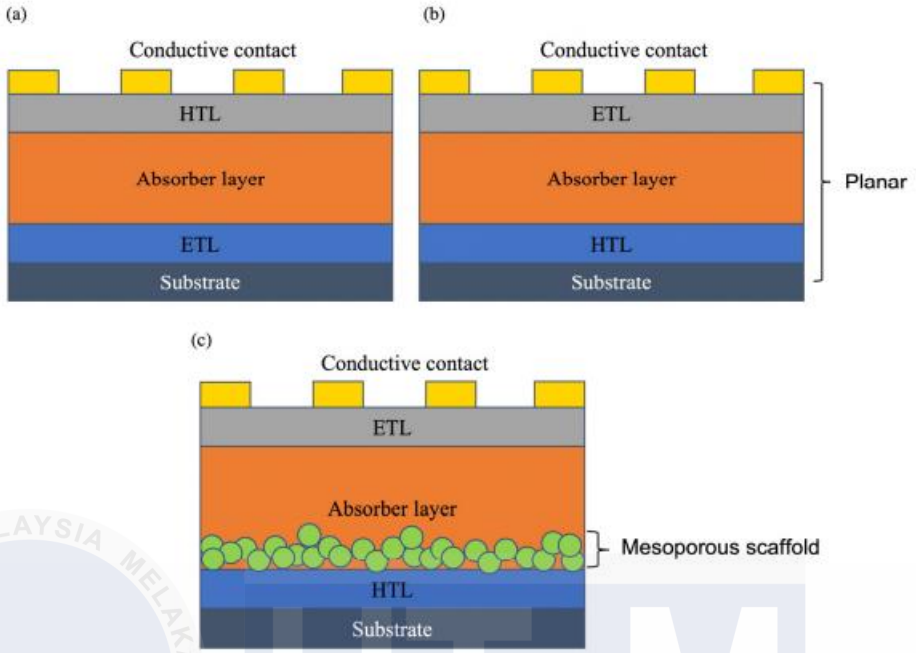

Figure 2.6: (a) Conventional PSC structure; (b) Inverted PSC structure; (c) mesoporous PSC structure [13]

A substrate layer, a thin layer of electron transport material (ETM), a perovskite absorber layer, a thin layer of hole-transporting material (HTM), and a final layer of conductive contact make up the traditional PSC structure, which is represented by figure 3(a). This structure is the most often used structure. TiO_2 is frequently used for the ETM layer and fluorine- or indium-doped tin oxide for the substrate layer. The HTM layer, which is usually composed of spiro-OMeTAD, is positioned between the ETM and HTM layers, and the perovskite absorber layer. Over the HTM layer is put the last layer of conductive contact. The traditional PSC structure has the benefit of being highly efficient and simple to construct [13]. However, oxygen and moisture can cause it to deteriorate.

The ETM and HTM layers are arranged in the opposite order in the inverted PSC structure (Figure 3b), which is comparable to the regular PSC structure. The perovskite

absorber layer is positioned between the HTM and ETM layers, with the ETM layer placed on top of the HTM layer. Because the perovskite layer is exposed to less oxygen and moisture than in the typical PSC structure, the inverted PSC structure has the advantage of being more stable. Nevertheless, compared to the traditional PSC structure, it is less efficient and more difficult to construct.

Unlike the conventional and inverted PSC designs, the mesoporous PSC structure (Figure 3c) employs a mesoporous TiO_2 scaffold structure rather than a planar architecture. Because of its greater surface area, the mesoporous structure facilitates more effective light absorption and electron transport. Nevertheless, compared to the traditional PSC structure, it is less efficient and more difficult to construct.

All things considered, the three distinct images above offer a succinct and clear visual depiction of the various PSC architectures and highlight the benefits and drawbacks of each design. PSC structure selection is based on the intended performance parameters and the application.

2.8 Development of flexible perovskite solar cells by the low-temperature fabrication of TiO_2 electron transport layers

The paper by Mohammed Al Shameili et al. (2020) explored a novel approach to the fabrication of flexible perovskite solar cells. The authors presented a method for fabricating TiO_2 electron transport layers (ETLs) at low temperatures, which can be applied to flexible substrates[14]. Moreover, the authors proceeded to explain on how they used low-temperature TiO_2 ETLs to create bendable perovskite solar cells. The deposition of TiO_2 layers on different flexible substrates using spin-coating and annealing processes was just one example of the extensive information they provided on the materials and techniques utilized in their research. The findings

used a variety of characterization methods, including as scanning electron microscopy, X-ray diffraction, and photoluminescence spectroscopy, were also included in the publication. The main conclusions and ramifications of the study were summarized in the paper's conclusion. The authors asserted that there is tremendous promise for the creation of low-cost and effective solar energy conversion technologies with their method of synthesizing flexible perovskite solar cells by utilizing low-temperature TiO_2 ETLs.

2.9 Comparative Study on Perovskite Solar Cells Using Inorganic Transport Layers

Next, the paper by Iqbal Kabir et al. (2019) presented a comparative study of perovskite solar cells with inorganic transport layers. The authors explored the effects of different inorganic transport layers on the efficiency and stability of perovskite solar cells. The perovskite solar cell concept and its potential for low-cost, high-efficiency solar energy conversion was introduced at the outset of the study. The significance of the transport layers in perovskite solar cells and the difficulties in improving them for effective charge transport were emphasized. The examination of perovskite solar cells in comparison to those with inorganic transport layers produced better device performance in terms of stability and efficiency, according to the publication. They added that the performance of perovskite solar cells can be considerably affected by the choice of inorganic transport layer[15]. The authors proposed that the inorganic transport layer optimization for perovskite solar cells can be guided by the findings of their investigation.

2.10 Investigate of TiO_2 and SnO2 as electron transport layer for perovskite solar cells

Furthermore, the paper by Ahmed A. Assi et al. (2020) explores the use of TiO_2 and SnO2 as electron transport layers (ETLs) in perovskite solar cells. The authors investigated how these ETLs affected the performance of perovskite solar cells and offer crucial information for these devices' optimization. These cells have a perovskite substance in the active layer that absorbs light and produces charge carriers. ETLs are a key element in achieving efficient charge transport, which is essential for the performance of perovskite solar cells. While preventing charge carrier recombination, ETLs offer a route for electrons to travel from the perovskite layer to the electrode[16].

The need for greater research on the optimization of ETLs in perovskite solar cells is one potential research gap that this study focuses to fill. Even though earlier studies investigated the use of various materials for ETLs, further study is still needed to determine how to best optimize these layers for increased performance and stability. More study is required regarding the effect of ETL shape, thickness, and surface characteristics on the functionality of perovskite solar cells.

Table 2.1: Previous study using TiO_2 as ETL layer

Solar cell structure	V_{OC} (mV)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)	Reference
PEDOT: PSS/$MASnl_3$/TiO_2	1.06	33.0	73.1	25.5	[17]
FTO/TiO_2/$(FA)_2BiCuI_6$/spiro-MeOTAD/Au	0.94	32.95	80.73	24.98	[18]
ITO/ZnO(i)/CdS/CBT (S, Se_3)/Mo/Glass	0.867	16.986	49.63	7.31	[19]
FTO/ZnO/SnO_2/TiO_2/$Ch_3NH_3PbI_3$/NiO_x	0.9995	22.98	74.57	17.13	[20]
FTO/NiOx/$Ch_3NH_3PbI_3$/ETM (varied)	1.059	21.022	77.06	17.16	[21]
FTO/TiO_2/$Cs_3Bi_2I_9$/Spiro-MeOTAD	1.22	12.19	77.73	11.54	[22]
FTO/CuSCN/ $Ch_3NH_3PbI_3$/TiO_2	1.1	28.9	82.08	28.9	[23]
FTO/TiO_2 /$Cs_3Bi_2I_9$/HTL/Au	0.92	21.91	68.05	13.69	[24]
FTO/TiO_2/ Cs_2BiCuI_6/SpiroOMeTAD	1.2787	21.1	83.21	22.02	[25]
FTO/TiO_2/Cs_2TiBr_6/P_3HT/Au	0.93	4.35	59.54	2.41	[26]

CHAPTER 3

METHODOLOGY

This chapter describes the research methodology for the study and explains the rationale for selecting the particular methodology.

3.1 Overview

This analysis consists of one major part, which is simulation. The simulation is carried out by using SCAPS-1D software. The PSC structure is investigated throughout various aspects, such as the working temperature, the thickness of the ETL layer, doping density, and defect density. The I-V characteristics that have been gathered are used to evaluate the overall performance of the system. The figure below shows a flowchart for this project.

3.2 Flowchart

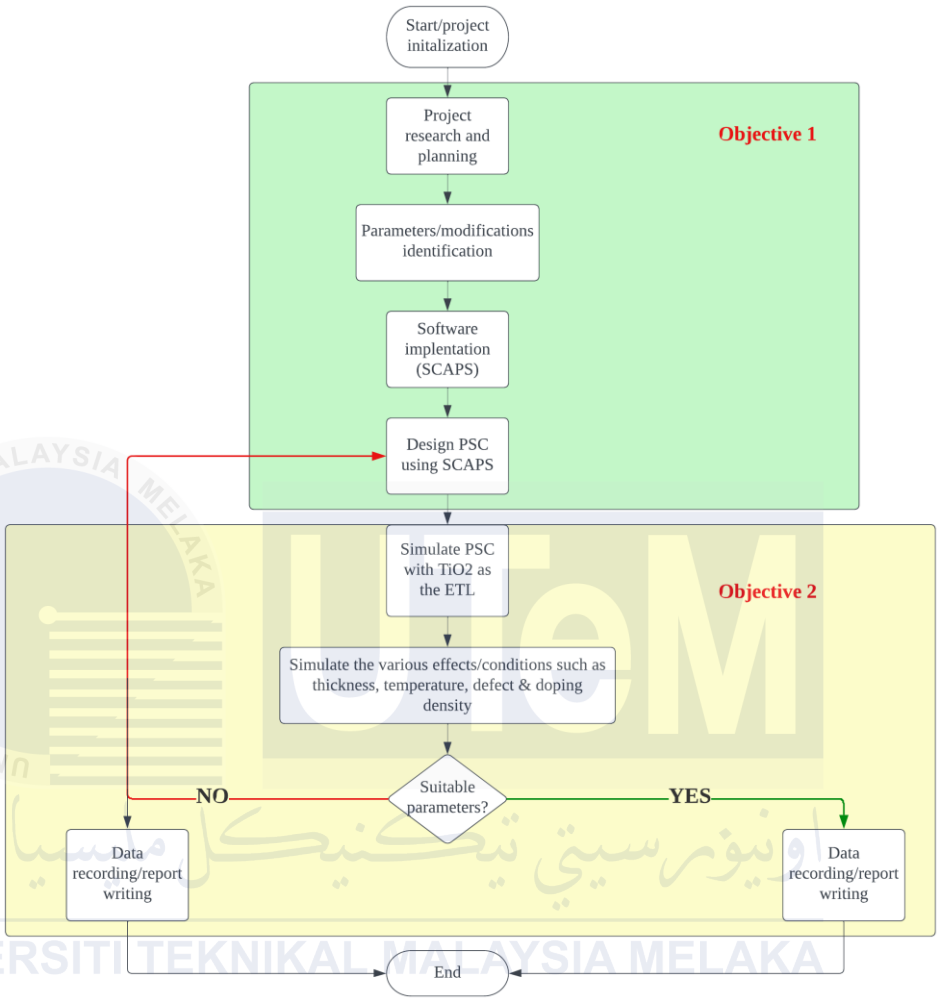

Figure 3.1: Flowchart for this project

Based on Figure 3.1, the project begins with the project initialization phase, in which the individual establishes the project's goals, objectives, and scopes. It entails identifying the important stakeholders, setting project deadlines and milestones, allocating resources, and putting together a project plan. Subsequently, the project is the focus of extensive investigation to gather information and evaluate previously held beliefs. This include reviewing relevant literature, reviewing previous studies, and being aware of novel discoveries. Based on the study results, a comprehensive project plan is developed that outlines the specific tasks, methods, and deadlines required to

meet the project's goals. After the project strategy has been established, the focus shifts towards gathering, arranging, and analyzing the required data. This involves gathering pertinent data, conducting statistical analysis, using data mining tools, and deriving insightful conclusions. Through the identification of patterns, trends, and correlations throughout the data analysis phase, the project can be run with more informed choices. The SCAPS (Semiconductor Device Modelling Software) system is implemented during the software development phase. This software's simulation and modelling capabilities help with the design and optimization of different electronic components. To make sure the software operates properly, the implementation process could involve development, testing, debugging, and integration. Moving on to the next element in the flowchart which is “Design PSC using SCAPS”, a Power Semiconductor Component (PSC) is designed based on the project specifications using the SCAPS software. The SCAPS tool makes it possible to create precise models, enabling engineers to optimize the design parameters and evaluate the PSC's performance under various operating scenarios. This iterative method entails tweaking the design until the outcome can be considered as desirable. Titanium dioxide (TiO_2) is used to simulate ETL in this phase of the procedure. TiO_2 serves as the reactive material in the ETC process, which uses heat to start chemical reactions. The simulation aids in forecasting TiO_2 performance in the ETC process, analyzing TiO_2 behavior, and refining operational parameters for effective manufacturing. It is crucial to accurately record all experimental data, simulation findings, and observations throughout the project. Documenting the results, analyzing the data gathered, and creating an extensive report are all included in the project implementation. The report provides an invaluable resource for future reference and dissemination of the project

results by summarizing the study's methodology, findings, conclusions, and recommendations.

3.3 Software Used

3.3.1 SCAPS-1D

Using LabWindows/CVI from National Instruments, Professor Marc Burgelman of Gent University's Department of Electronics and Information Systems (ELIS) developed SCAPS-1D, a graphical simulation application for solar cells [27]. One of the many unique features of SCAPS is its capacity to simulate up to seven different layers with non-routine measurements (C-V, C-f). It may ascertain several factors, including spectrum response, energy bands, AC properties, JV curve, and defect density, by solving three fundamental semiconductor equations [28]. The effect of defect density, thickness, absorber layer doping density, carrier diffusion length, and electron affinity of ETL layers on PSC performance is examined using the SCAPS-1D software [29]**.** With it, one may create a p-n junction, add contacts, and model the bandgap energy diagram and I-V curve of a solar cell. A straightforward program/platform called SCAPS can be used for both research and teaching. The activity panel of SCAPS-1D is shown in **Figure 3.2**. It illustrates the working point, illumination, parameter simulation, and numerous other ongoing actions.

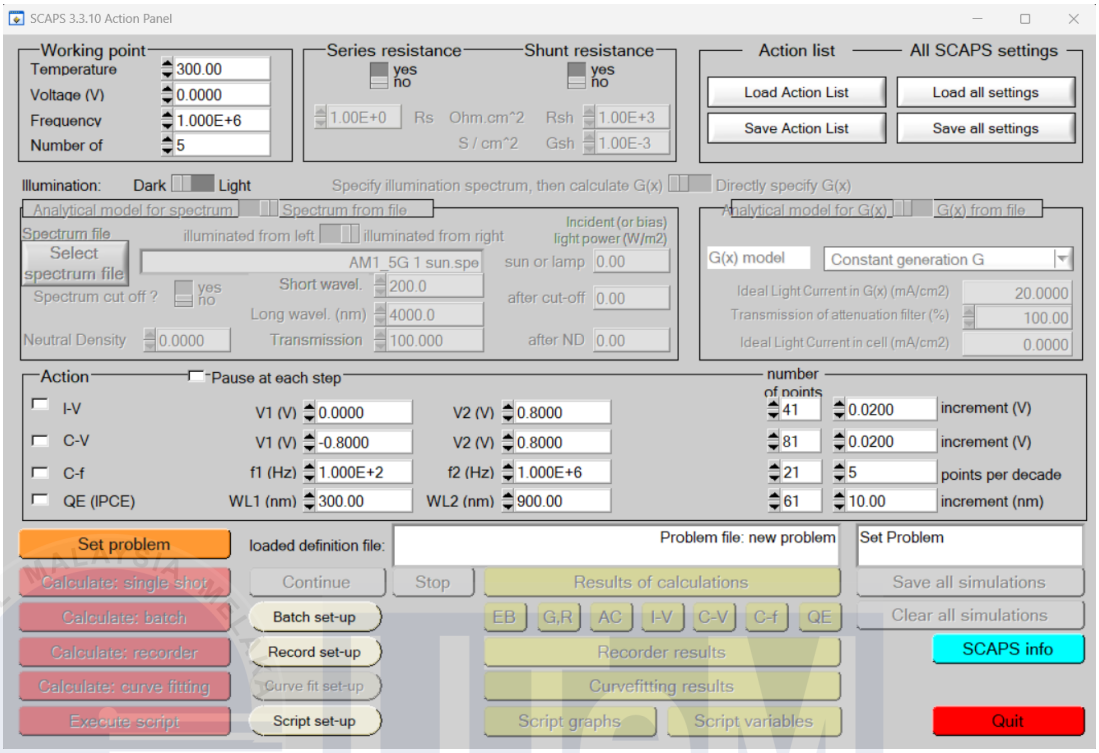

Figure 3.2: Action Panel of SCAPS-1D

The figure above shows the initial screen when SCAPS is launched. This initialization screen is said to be the Action Panel. The first procedure would be to press the “set problem” button to set the layers of the PSC according to our desire.

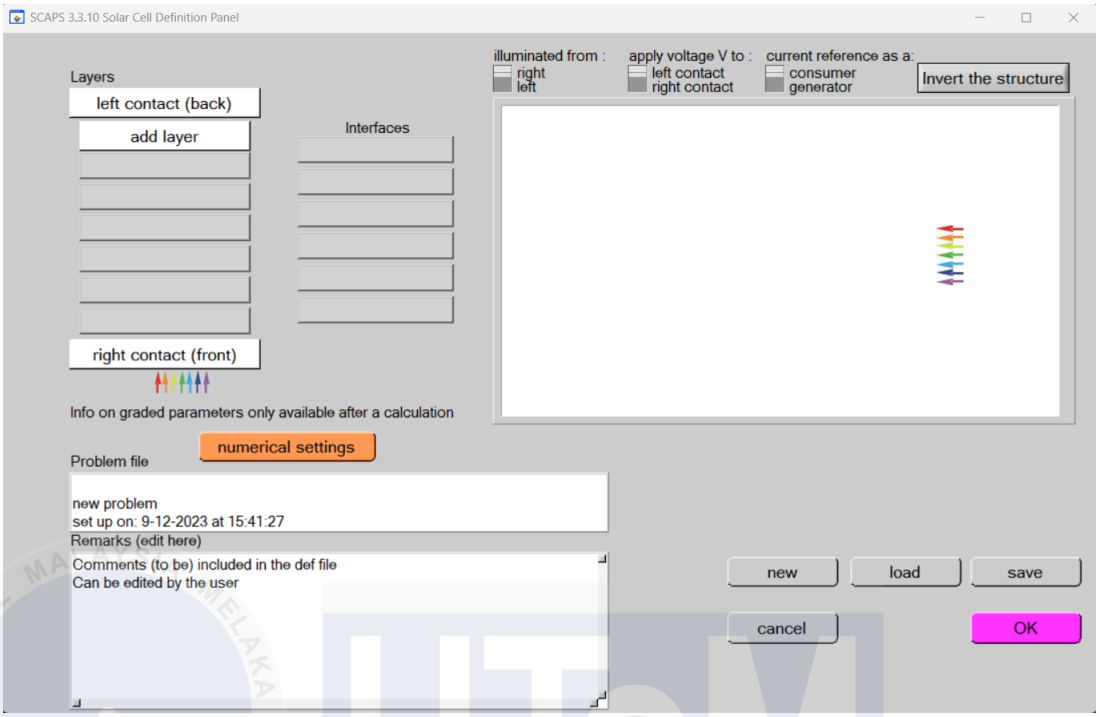

Figure 3.3: Solar Cell Definition Panel

When the 'set problem' button is selected, the application now displays an interface as shown in figure 3.3 above. This interface allows users to customize or randomize their choice of materials to make up the PSC layers that are needed to be ran through simulation in the coming steps. Not only that, this interface is known as the Solar Cell Definition Panel and it can also alter the defects for each layer within the cell. Lastly, the file from this definition panel will be saved as ".def" format files.

3.3.2 Implementation of TiO_2 Simulation in SCAPS-1D

For this study, PSC device model is made up of five layers. The said layers are ITO, TiO_2, $CH_3NH_3SnI_3$ and CUI in the respective PSC layer. CUI is the front contact of the PSC while $CH_3NH_3SnI_3$ acts as an absorber layer. Not only that, TiO_2 is the ETL and CUI is the HTL in the setup that accumulates into forming the PSC. The back contact of the PSC is ITO or glass. The said formation of the layer arrangement in the SCAPS-1D software is shown in figure 3.4.

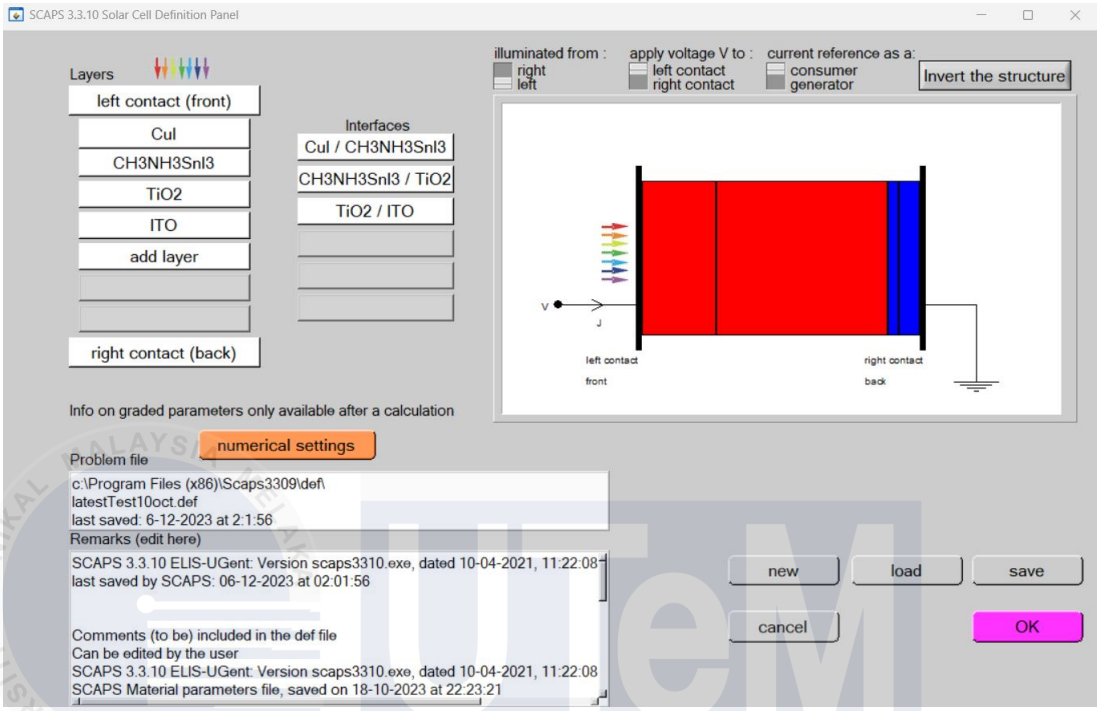

Figure 3.4: PSC lead-free layers structure set-up

The PSC efficiency has been improved by focusing on several TiO_2-related properties. Some of the parameters regulated regarding the TiO_2 layer are thickness, concentration, density, photovoltaic cell operating temperature, and the defect interface.

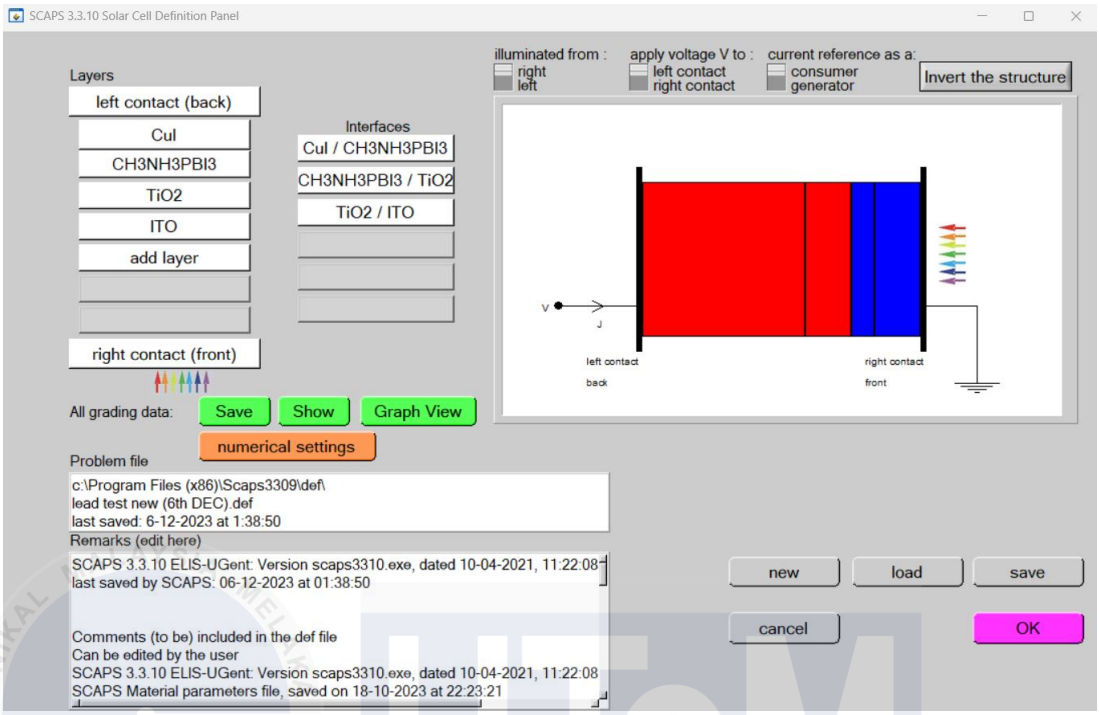

Figure 3.5: PSC lead-based layers structure set-up

Figure 3.5 shows a lead-based PSC structure that is using $CH_3NH_3PBI_3$ as the absorber layer. Other layers remain as constant as the one shown in figure 3.4. This is to contrast the PSC structure between lead-free and lead-based to be used later in the analysis and results part in this thesis.

Table 3.1: Input parameter of numerical analysis for PSC structure

Parameters	ITO [30]	TiO_2 [31]	$CH_3NH_3SnI_3$	CuI	$CH_3NH_3PBI_3$
Layer thickness, d (nm)	100	50 (variable)	800	350	100
Bandgap energy, Eg (eV)	3.3	3.2	1.3	3.1	1.55
Electron affinity, (eV)	4.1	3.9	4.2	2.1	3.9
Dielectric permittivity, ε (relative)	2	9	10	6.5	30
Conduction Band density of states, NC (cm^{-3})	2.0×10^{20}	1.0×10^{19}	1.0×10^{18}	2.5×10^{19}	$2.2x10^{18}$
Valence Band density of states, NV (cm^{-3})	1.8×10^{19}	1.0×10^{19}	1.0×10^{18}	2.5×10^{19}	$1.8x10^{19}$
Electron thermal velocity, Ve (cm/s)	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	$1.0x10^{7}$
Hole thermal velocity, Vh (cm/s)	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	$1.0x10^{7}$
Electron mobility, μe (cm^2 /Vs)	1.0×10^{19}	2.0×10^{1}	1.6	1.0×10^{2}	2
Hole mobility, μh (cm^2 /Vs)	7.5×10^{1}	1.0×10^{1}	1.6	4.39×10^{1}	2
Density of donor, ND (cm^{-3})	1.0×10^{19}	5.0×10^{17}	0	0	0
Density of acceptor, NA (cm^{-3})	0	0	1.0×10^{17}(Variable)	1.0×10^{18}	$1.0x10^{17}$

3.3.3 Investigating Procedure

The critical parameter values of TiO_2 as an ETL were investigated to achieve the highest efficiency for PSC. A defect interface between each layer, the thickness of TiO_2, the doping density of TiO_2 and CuI, the operating temperature of the solar cell, and all these factors need to be examined and considered.

3.3.3.1 Investigating the modifications of temperature in TiO_2

The solar cell's power conversion efficiency is influenced by its operating temperature. In this study, the temperature ranges from 300 K to 400 K to achieve the best power conversion efficiency. PSC's temperature is expressed in Kelvin.

3.3.3.2 Investigating the modifications of thickness in TiO_2

By altering the layer thicknesses within the same structure, the thickness analysis for ETL TiO_2 is conducted. In this study, the only changes made to a simulation are to the ETL layer.

3.3.3.3 Investigating the modifications of concentration density in TiO_2

In most circumstances, the more doping, the lower the conductivity due to increasing carrier concentration. The doping density occurs in the ETL and HTL layers. The ETL layer contains ND, whereas the HTL layer has NA. In this study, the values of ND and Ne ranged from 10^{14} to 10^{20} cm^{-3}.

3.3.3.4 Investigating the modifications of defect density in TiO_2

This research only investigated one kind of defect density interface which is a neutral one. One of the potential problematic interface layers is the imperfection at the interface between the TiO_2 and $CH_3NH_3SnI_3$ layers. The neutral defect density is varied from 1×10^{10} to 1×10^{20} cm^{-3}.

CHAPTER 4

RESULTS AND DISCUSSION

This chapter will go over the results acquired as well as the theory associated with the project that was completed successfully. To improve solar cell performance and cell efficiency, various characteristics are observed and measured.

4.1 Analysis of TiO_2 on perovskite

Using the SCAPS-1D software, a numerical simulation is run as the initial stage in the investigation. To get the maximum efficiency, the parameters of each structured layer are examined and optimized. The J-V curve acquired in this simulation was used to record and analyze the solar cell's efficiency value (PCE), open-circuit voltage (V_{OC}), short circuit current (J_{SC}), and fill factor (FF).

4.1.1 Analysis of working temperature

One of the crucial factors that might significantly affect the perovskite solar cell's photovoltaic performance is its working temperature. The temperature ranges shown in this simulation span from 300 K to 400 K, with 20 K steps or gaps between each value. Table 4.1 below indicates the fixed-parameter value in plotting the temperature graph. The data and graph from the Perovskite simulations are included in Table 4.2 and Figure 4.1 respectively.

Table 4.1: Constant parameter value for working temperature analysis

Parameter	TiO_2
Thickness of TiO_2 (nm)	50
Thickness of CuI (nm)	350
Doping donor density	10^{17}
Doping acceptor density	0

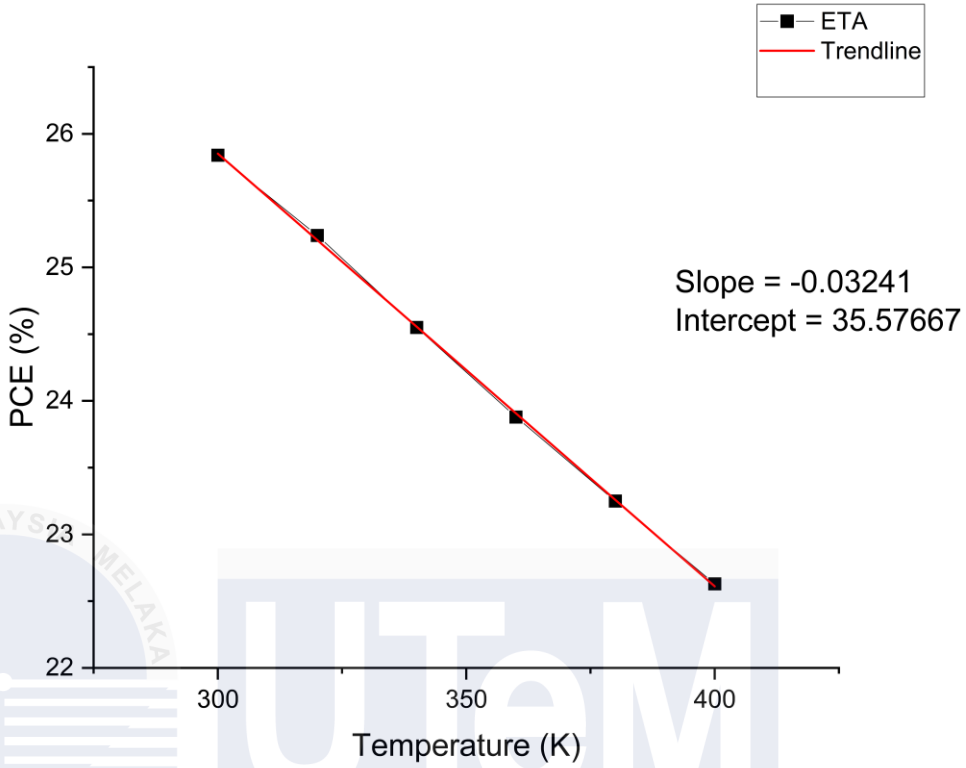

Figure 4.1: The analysis of efficiency based on the variation of working

Table 4.2: The analysis of efficiency based on the variation of working temperature

Working temperature (K)	VOC	JSC	FF (%)	PCE (%)
300	1.0137	30.152344	84.54	25.84
320	0.995	30.186104	84.03	25.24
340	0.9732	30.252549	83.38	24.55
360	0.9498	30.364733	82.81	23.88
380	0.9259	30.533393	82.24	23.25
400	0.9021	30.763859	81.53	22.63

Based on figure 4.1 above, the graph obtained shows a downwards trend in the efficiency (PCE) as the operating temperature increase to the parameters that has been set. The inclination or the gradient of the downwards trend is 0.03241 %/Kelvin. All the parameters except J_{SC}, which are laid out in the table 4.2 above, shows a decreasing trend as the temperature rises. Meanwhile, J_{SC} shows a slight increase in its trend value. This is because, the material's carrier concentration, charge mobility, resistance and bandgap were all affected by the high operating temperatures, resulting in a shift in the PV's key properties [32]. Moreover, the rate of internal carrier recombination is particularly accelerated by the higher carrier concentration in the semiconductor that is produced by a higher operating temperature. An increase in reverse saturation current causes a decrease in VOC.

4.1.2 Analysis of the variation of TiO_2 thickness

In this analysis, the thickness of TiO_2 is the varied parameter, which ranges from 5 nm to 250 nm. Table 4.3 below indicates the fixed-parameter value in plotting the thickness graph against the efficiency (PCE). On the other hand, table 4.4 shows the data obtained from the result of varying the ETL thickness.

Table 4.3: The constant set parameter value for ETL thickness analysis

Parameter	TiO_2
Working temperature (K)	300
Thickness of CuI (nm)	350
Doping donor density (cm^{-3})	10^{17}
Doping acceptor density (cm^{-3})	0

Table 4.4: The analysis of efficiency based on the variation of ETL thickness

ETL Thickness (nm)	VOC	JSC	FF (%)	PCE (%)
5	1.0138	30.095559	84.34	25.73
25	1.0137	30.063731	84.73	25.82
50	1.0137	30.152919	84.54	25.84
75	1.0137	30.150238	84.54	25.84
100	1.0137	30.145839	84.54	25.83
125	1.0137	30.14073	84.54	25.83
150	1.0137	30.135022	84.54	25.83
175	1.0137	30.128809	84.54	25.82
200	1.0137	30.122122	84.55	25.82
225	1.0137	30.115078	84.55	25.81
250	1.0137	30.107773	84.55	25.80

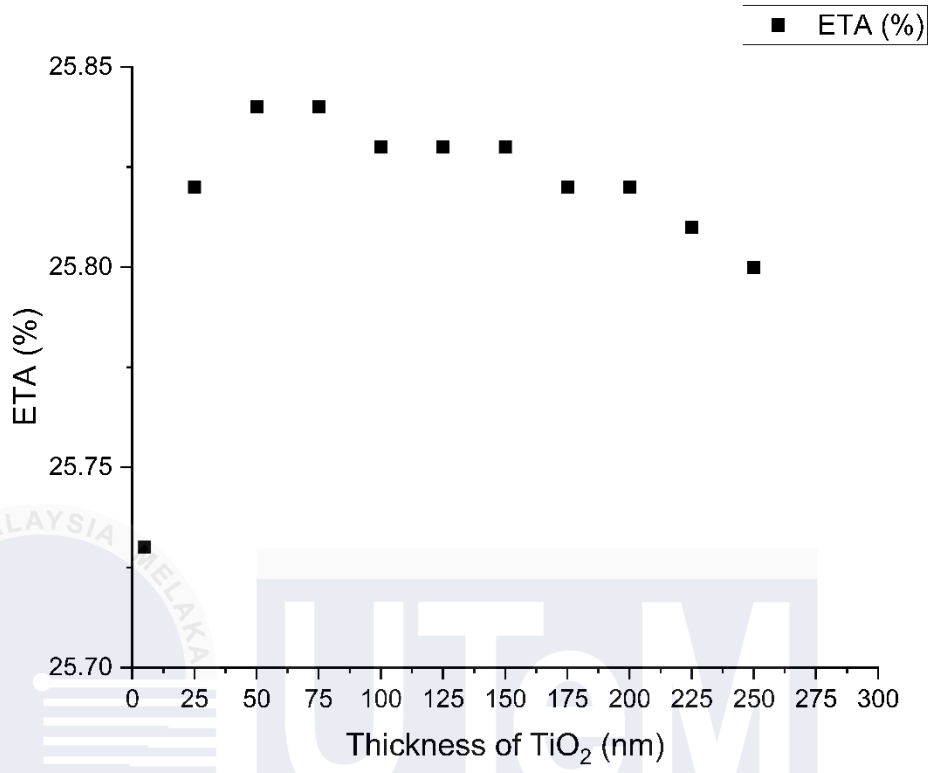

Figure 4.2: The analysis of efficiency based on the variation of ETL thickness

Based on figure 4.2, the graph obtained shows the increase in ETL thickness affect the attenuation of PCE. Additionally, it lowers the voltage and current of the cell, however the difference is not enormous. The highest PCE value is around 31.00% at approximately 25nm, 50 nm and 75 nm respective thicknesses of TiO_2, after which it begins to decline. The reason for the decrease in PCE with increasing TiO_2 thickness is that as the material becomes thicker, less light is absorbed by it, which reduces the quantity of electrons produced. The power conversion efficiency (PCE) of the solar cell decreases because of the said drop in electron generation. There are numerous effects that can result from PCE attenuation caused by a thick ETL. For instance, a thicker ETL may make it take an electron longer to reach the ITO, increase the series resistance of the device, and reduce the fill factor, all of which can impair solar cell efficiency. Additionally, the electron tends to lower the V_{OC} and increase the

recombination rate. Since more photons can flow through the ETL layer and be absorbed in the absorber layer, thinner ETL is preferred. It goes without saying that longer charge carrier mobility is caused by greater ETL/HTL thickness values. By increasing the likelihood of carrier recombination, the generated photo current and, thus, the PCE value will be further reduced [20]. In summary, thickness of TiO_2 ranging between 25 to 75 nm is considered optimum thickness value.

4.1.3 Analysis of the variation of Doping Donor Density

Next, the analysis of doping density is then varied from 10^{14} cm^{-3} to 10^{19} cm^{-3}. Table 4.5 shows the constant parameters that are used to analyze and plot the doping donor density, whereas Table 4.6 displays and records the data acquired from the simulation.

Table 4.5: The constant set parameter value for doping donor density

Parameter	TiO_2
Thickness of TiO_2 (nm)	50
Thickness of CuI (nm)	350
Doping donor density (cm^{-3})	10^{17}
Temperature (K)	300

Table 4.6: Analysis of efficiency based on the variation of doping donor density

Doping donor density (cm^{-3})	VOC	JSC	FF (%)	PCE (%)
10^{14}	1.0146	29.304558	67.32	20.02
10^{15}	1.0146	29.307167	67.53	20.08
10^{16}	1.0145	29.333012	69.65	20.73

10^{17}	1.0139	29.567285	84.02	25.19
10^{18}	1.0137	30.2146	84.43	25.86
10^{19}	1.0136	30.119145	84.43	25.78

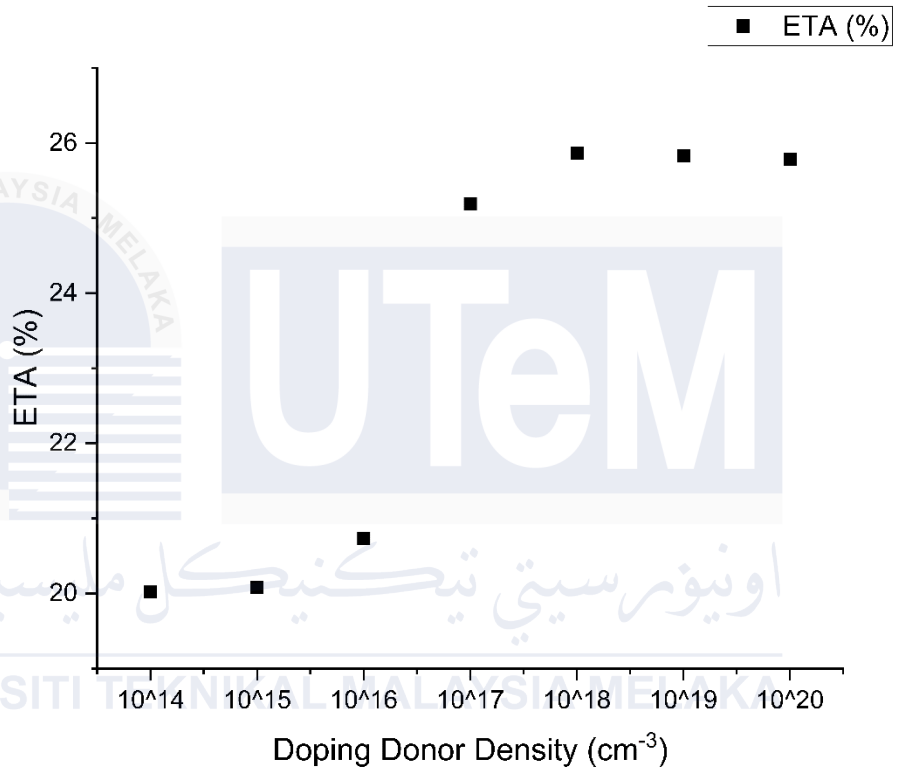

Figure 4.3: The analysis of efficiency based on the variation of doping donor

As the doping acceptor density increases, the figure above shows how the device's efficiency increases. According to Figure 4.3, efficiency increases as donor density does. This is because, increasing doping is equivalent to adding more impurities to a semiconductor to alter its structural, optical, and electrical characteristics [33]. As a result, the semiconductor will produce more free charge as the number of impurities increases. An increase in free charge suggests that more current is passing through the

system simultaneously, which lowers the series resistance. Therefore, there has been an improvement in efficiency.

4.1.4 Analysis of the variation of Defect Density at the interface

Furthermore, the variation of defect density is involving the layers of $CH_3NH_3SnI_3/TiO_2$. It is varied from 10^{10} cm^{-2} to 10^{20} cm^{-2}. Figure 4.4 demonstrates the graph obtained for the defect density. Meanwhile, Table 4.7 shows the parameters that are kept constant for the use of this analysis. The analysis of efficiency based on different defect densities at $CH_3NH_3SnI_3/TiO_2$ can be referred to in Table 4.8.

Table 4.7: The constant set parameter value for defect density analysis

Parameter	TiO_2
Thickness of TiO_2 (nm)	50
Thickness of CuI (nm)	350
Doping donor density (cm^{-3})	10^{17}
Temperature (K)	300

Table 4.8: Analysis of efficiency based on the variation of defect density at $CH_3NH_3SNI_3/TiO_2$

Defect density at $CH_3NH_3SnI_3/TiO_2$	VOC	JSC	FF (%)	PCE (%)
10^{10}	1.1143	33.171182	83.86	30.99
10^{12}	1.0137	30.152344	84.54	25.84
10^{14}	1.0111	30.078062	84.64	25.74
10^{16}	1.0108	30.069817	84.65	25.73
10^{18}	1.0108	30.069803	84.65	25.73

10^{20}	1.0108	30.069802	84.65	25.73

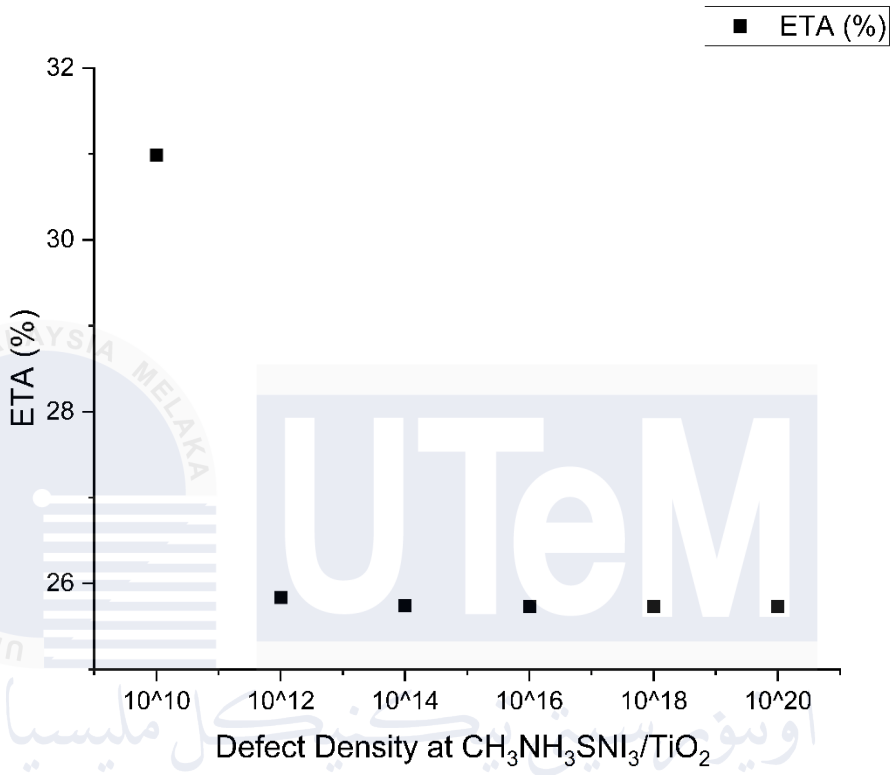

Figure 4.4: The variation of defect density at $CH_3NH_3SNI_3/TiO_2$

The figure above depicts that the depreciation can only be seen from 10^{10} onto the next values. From there, it can be said the efficiency value remains somewhat constant as the depreciation value is not significant from 10^{12} to 10^{20}. The performance of the PSC increases due to the result of reduced carrier loss owing to recombination because of low defect density. Defect density depends on the quality of the absorber layer. Higher defect density is the result of low quality. Because of this, the efficiency of the perovskite layer decreases as recombination of electron-hole pairs increases [34].

4.2 Analysis of efficiency based on optimum value for all parameters

Table 4.9 below lays out the optimum value for all parameters achieved from the simulation analysis. The J-V curve of optimized PSC structure with TiO_2 as an ETL is shown in Figure 4.5.

Table 4.9: The optimum parameter of the simulated PSC structure

Parameters	TiO_2
Thickness of TiO_2 (nm)	50
Working Temperature (K)	300
Density of donor, ND (cm^{-3})	$5.0x10^{17}$
Density of acceptor, NA (cm^{-3})	0
Defect at $CH_3NH_3PBI_3/TiO_2$ interface (cm^{-2})	$1.0x10^{18}$
Open-circuit voltage, V_{OC} (V)	1.0137
Short-circuit current density, J_{SC} (mA/cm^2)	30.152344
Fill factor (%)	84.54
PCE (%)	25.84

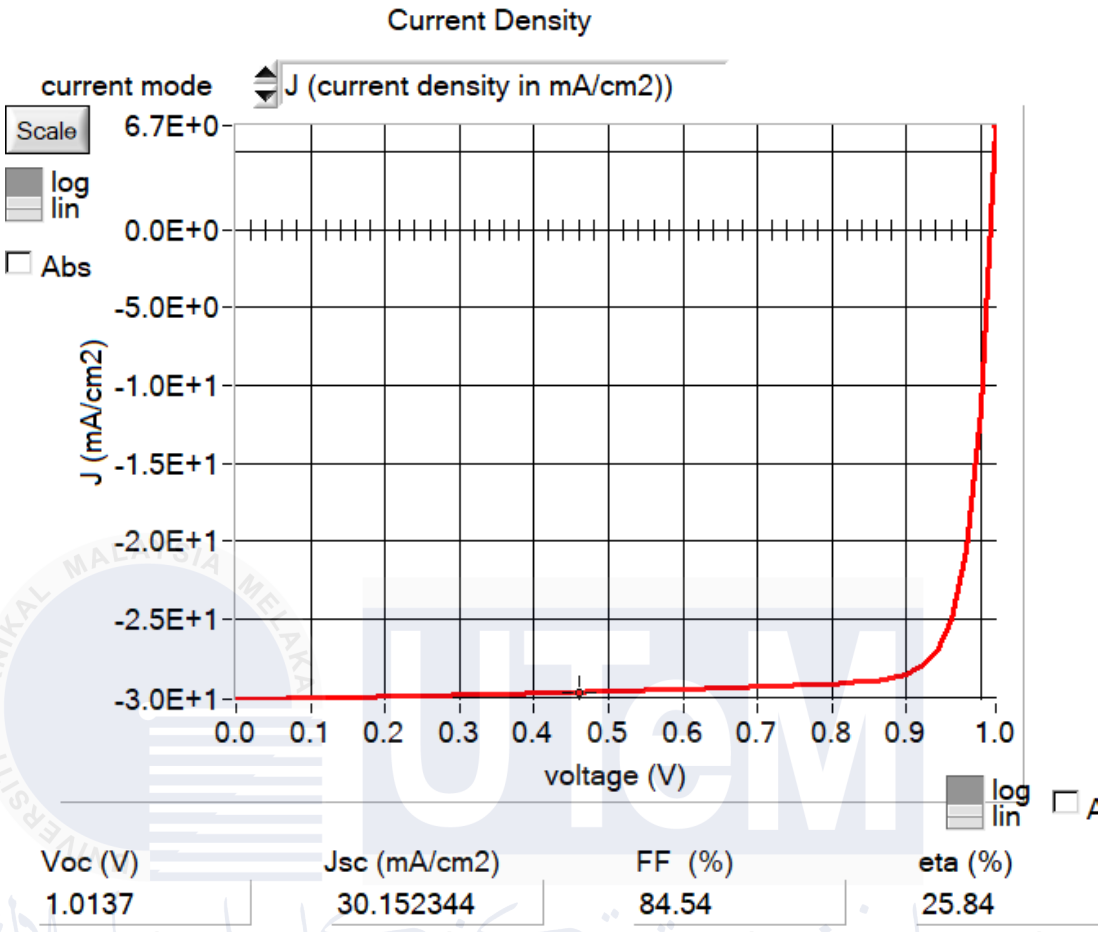

Figure 4.5: J-V curved for the optimized lead-free PSC structure

Based on Table 4.9, the simulation analysis findings exhibits that TiO_2 produced the optimized efficiency by replacing all of the parameters with the optimal value. The PCE achieved is 25.84%, V_{OC} of 1.0137 V and J_{SC} of 30.152344 mA/cm^2.

4.3 Analysis of efficiency for lead-based PSC

The simulation done in subsection 4.2 is compared closely with the simulation findings of lead-based PSCs. This is to contrast this project and other projects that are using lead-based materials or substances in their research.

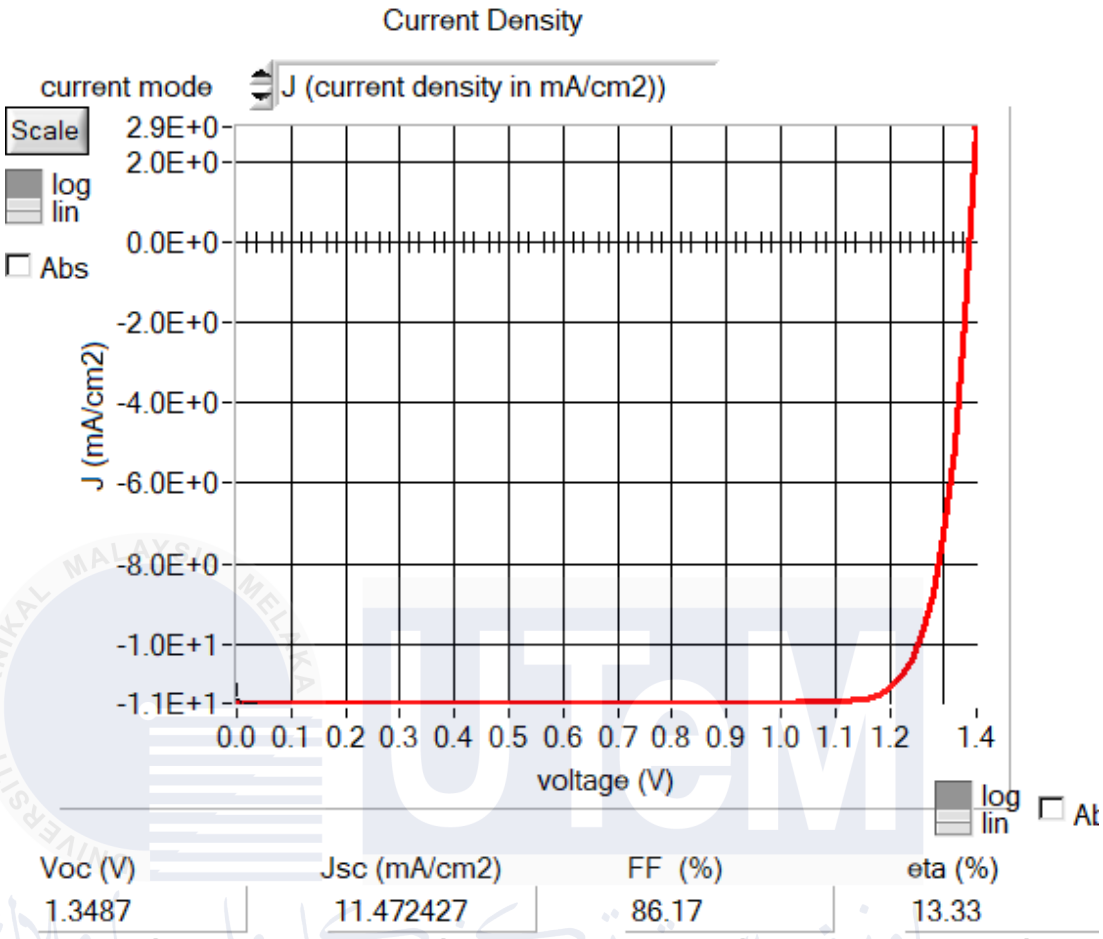

Figure 4.6: J-V curve for the lead-based PSC structure

Based on figure 4.6, the PCE achieved is 13.33%, V_{OC} of 1.3487 V and J_{SC} of 11.472427 mA/cm^2. The lead-based PSC structure simulation analysis is done to illustrate the contrast between the lead-free and lead-based PSC structure.

4.4 Is the project relevant to sustainability and is it environmental friendly?

The project of using TiO_2 as the ETL for perovskite solar cells relate closely with Sustainable Development Goals (SDG) goal number 7.

Figure 4.7: SDG Goal 7

This research may contribute to achieve SDG 7 by offering an affordable and sustainable energy source. The initiative can contribute to lowering energy poverty and expanding access to clean energy by utilizing PSCs. The efficiency of the devices can be increased by using TiO_2 as an ETL in PSCs, which can lower the cost of solar energy and increase its accessibility for those in need.

In conclusion, the project's use of TiO_2 as an ETL in PSCs can support SDG 7 by offering a cheap and sustainable energy source that can aid in lowering energy poverty and expanding access to clean energy.

CHAPTER 5

CONCLUSION AND FUTURE WORKS

5.1 Conclusion

The third generation of solar cells is represented by perovskite solar cells. There are three primary parts to it, which are the absorber, HTL, and ETL. To improve the efficiency of the PSC, various analysis and investigations have been carried out in terms of research and simulation. Furthermore, TiO_2 is one of the most promising materials for an ETL that contains favorable attributes such as wide optical band gap (up to 3.2 eV), good transmittance feature, and it can be processed by the low-temperature method.

In this study, a PSC structure that is made up of ITO/TiO_2/absorber layer/CuI has been analyzed by using the SCAPS-1D software. the absorber layer is varied between two materials, which are $CH_3NH_3SnI_3$ (lead-free) and $CH_3NH_3PBI_3$ (lead-based). This

analysis's primary goal is to use TiO_2 as an ETL to develop a PSC structure. The working temperature of a solar cell, the thickness of ETL, the dopant density of both HTL and ETL, and the defect density at the interface between the absorber and ETL are among the parameters that go into designing the best structure.

In the lead-free simulation analysis, the optimum efficiency obtained has the value of 25.84% at 300 K working temperature, 50 nm thickness of TiO_2, 0 cm^{-3} doping acceptor density, 10^{17} cm^{-3} doping donor density and 10^{14} cm^{-2} defect density. On the other hand, the simulation for the lead-based PSC structure obtained an efficiency of 13.33% with all the parameter settings being constant as the one listed for the lead-free PSC structure.

Despite their low cost and excellent efficiency, lead-based perovskite solar cells have found widespread use in the photovoltaic sector. But lead's toxicity poses a serious threat to both human health and the environment. Perovskite solar cells free of lead, on the other hand, are thought to be safer and more environmentally benign. Numerous non-toxic or low-toxic materials have been used in their development, some of which have demonstrated exceptional optoelectronic characteristics and device performance [4].

5.2 Future work

This work has been focusing on the simulation analysis of TiO_2 being the ETL for the perovskite solar cells. Therefore, fabrication should be carried out in the future. There are a few techniques that can be used in terms of carrying out the fabrication process. In the Chemical Deposition Bath (CBD) technique, it involves the deposition of a thin film of TiO_2 on a substrate by immersing it in a chemical bath containing a precursor solution of TiO_2. The precursor solution is then hydrolyzed to form a thin

film of TiO_2 on the substrate. Next, for a technique named as ‘Spin Coating’, a solution of TiO_2 is spin-coated onto a substrate to form a thin film. The substrate is then annealed to remove any residual solvent and to densify the TiO_2 film. For the Sputtering technique, a thin film of TiO_2 is deposited on a substrate by bombarding a TiO_2 target with high-energy ions. The TiO_2 atoms are then ejected from the target and deposited on the substrate. There are several techniques that can be used to fabricate TiO_2 but it must be first understood on the details of each respective techniques and which technique is the most suitable for this project.

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