INTRODUCTION OF THIN LAYER OF GRAPHENE OXIDE (GO) AS HOLE TRANSPORT MATERIAL (HTM) FOR SOLAR CELL APPLICATION

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in fulfillment of the requirements for the degree of
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DEDICATION

This thesis is specially dedicated to my beloved parents Mr & Mrs Vincent Praboo, supportive supervisor Ts Dr Faiz Bin Arith and all my fellow batch mates that have guided me along the way in completing the report. Greatfull to have a supervisor that guides me and continous encouragement throughout the journey in completing the project.

ABSTRACT

Perovskite solar cells (PSCs) have made tremendous strides in device performance and power conversion efficiency (PCE), which has given the photovoltaic field as a whole a sense of accomplishment recently. The conventional structure of perovskite solar cells (PSCs) consists of many layers that are necessary for their operation. A perovskite layer for absorption and other layers for charge extraction and transport are the fundamental parts of a perovskite solar cell. The negative and positive charges are transported by these extra layers, which could be an electron-transport layer (ETL) or a hole-transport layer (HTL), respectively. Nonetheless, there are certain drawbacks on the current conventional structure of hole-transport material (HTM) used which has greater cost and requires equivalent dopants which eventually turned out to be Perovskite Solar Cells instability caused by the humidity. Therefore, implementing Graphene Oxide (GO) as a Hole Transport Material that offers both inexpensive and has a good Hole Transport Layer interface plays an essential role to attain high Perovskite Solar Cells performance. The design on introducing thin layer of graphene oxide (GO) on hole transport material (HTM) for perovskite solar cell is further analyzed. Regarding this, the aim of the research is to simulate the thin layer Graphene Oxide as Hole Transport Material (HTM) in perovskite solar cell using SCAPs simulator and to analyse the performance of thin layer Graphene Oxide (GO) as Hole Transport Material (HTM) for perovskite solar cell.

PENGENALAN LAPISAN NIPIS GRAPHENE OXIDE (GO) SEBAGAI BAHAN PENGANGKUTAN LUBANG (HTM) UNTUK APLIKASI SEL SOLAR

ABSTRAK

Sel suria Perovskite (PSC) telah mencapai kemajuan yang besar dalam prestasi peranti dan kecekapan penukaran kuasa (PCE), yang telah memberikan medan fotovoltaik secara keseluruhannya merasai pencapaian yang terbaru. Struktur konvensional sel suria perovskite (PSC) terdiri daripada banyak lapisan yang diperlukan untuk beroperasi. Lapisan perovskite untuk penyerapan dan lapisan lain untuk pengekstrakan dan pengangkutan cas adalah bahagian asas sel solar perovskit. Caj negatif dan positif diangkut oleh lapisan tambahan ini, yang masing-masing boleh menjadi lapisan pengangkutan elektron (ETL) atau lapisan pengangkutan lubang (HTL). Namun begitu, terdapat kelemahan tertentu pada struktur konvensional semasa bahan pengangkutan lubang (HTM) yang digunakan yang mempunyai kos yang lebih tinggi dan memerlukan dopan setara yang akhirnya menjadi ketidakstabilan Sel Suria Perovskite yang disebabkan oleh kelembapan. Oleh itu, melaksanakan Graphene Oxide (GO) sebagai Bahan Pengangkutan Lubang yang menawarkan kedua-dua murah dan mempunyai antara muka Lapisan Pengangkutan Lubang yang baik memainkan peranan penting untuk mencapai prestasi Sel Suria Perovskite yang tinggi. Reka bentuk untuk memperkenalkan lapisan nipis graphene oxide (GO) pada bahan pengangkutan lubang (HTM) untuk sel solar perovskite dianalisis selanjutnya. Sehubungan dengan ini, tujuan penyelidikan adalah untuk mensimulasikan lapisan nipis Graphene Oxide sebagai Bahan Pengangkutan Lubang (HTM) dalam sel solar perovskite menggunakan simulator SCAPs dan menganalisis prestasi lapisan nipis Graphene Oxide (GO) sebagai Bahan Pengangkutan Lubang (HTM) untuk sel suria perovskite.

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Firstly, I am grateful to God for granting me the resources needed to successfully complete this project. However, without the generous support and assistance of numerous people, the effort would not have been able to accomplish its objectives. I'd want to express my heartfelt gratitude to all of them as conscious effort was enabled in this research.

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TABLE OF CONTENT

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

a-Si	-	Amorphous silicon
Au	-	Gold
CdTe	-	Cadmium Telluride
$CH_3NH_3PbI_3$	-	Methylammonium lead halide
CIGS	-	Copper Indium Gallium Di-selenide
CIS	-	Copper Indium Selenide
Cm	-	Centimetre
$CsSnI_3$	-	Cesium Tin Triiodide
Cu_2O	-	Copper(I) Oxide
$CuCrO_2$	-	Copper Chromite
CuI	-	Copper(I) Iodide
CuO	-	Copper (II) Oxide
CuPc	-	Copper (II) Phthalocyanine
CuSCN	-	Copper(I) Thiocyanate
ETL	-	Electron Transport Layer
eV	-	Electron Voltage
FF	-	Fill Factor
FTO	-	Fluorine-doped Tin Oxide
GO	-	Graphene Oxide
HTL	-	Hole Transport Layer
HTM	-	Electron Transport Material
J_{SC}	-	Short-circuit Current

$MAPbI_3$	-	Methyl Ammonium Lead Triiodide
$MASnI_3$	-	Methyl Ammonium Tin Triiodide
MoO_3	-	Molybdenum Trioxide
NiO	-	Nickel Oxide
Nm	-	Nanometre
PCBM	-	Phenyl-C61-butyric acid methyl ester
PCE	-	Power Conversion Efficiency
PEDOT:PSS	-	Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate
PSC	-	Perovskite Solar Cell
PV	-	Photovoltaic
QE	-	Quantum Efficiency
rGO	-	Reduced Graphene Oxide
SCAPS	-	Solar Cell Capacitance Simulator
TiO_2	-	Titanium Dioxide
UTeM	-	Universiti Teknikal Malaysia Melaka
V_{OC}	-	Open-circuit Voltage
ZnO	-	Zinc Oxide

LIST OF SYMBOLS

δ	-	delta
ε	-	Epsilon
λ	-	Lambda
Ω	-	Ohm
ψ	-	Psi
Σ	-	Sigma

CHAPTER 1

INTRODUCTION

This chapter outlines the project's relevance, objectives, scope of work and problems statements. In this chapter, the project overview and problem statement will be discussed in relation to the difficulties in modelling the electron transport layer free for perovskite solar cell applications. By the chapter's conclusion, the report summary's outline is included.

1.1 Background

Solar energy is becoming more popular as a sustainable and ecologically beneficial energy source. Solar energy has a potential of 4,8 kWh/m^2 or equals to 112,000 GW (Priharti, Rosmawati and Wibawa, 2019). The main application of solar energy is electrical generation through a photovoltaic (PV) system. The photovoltaic sensor is a semiconductor device that changes light into electrical energy. The photovoltaic sensor ability to generate voltage is influenced by the amount of light that strikes it. The photovoltaic term refers to their capacity to produce voltage. The compound connects the electrons in the semiconductor material. The tiny energy particles known as photons make up electromagnetic radiation. The semiconductor material absorbs photons, which then energize the electrons and cause them to begin emitting.

The photovoltaic effect is the basis for converting light energy into electrical energy. When semiconductor materials are exposed to light, part of the light photons are absorbed by the semiconductor crystal, resulting in a considerable number of free electrons in the crystal. The primary driver behind photovoltaic effect power production is this. The fundamental building block of a system that uses the photovoltaic effect to generate electricity from light energy is a photovoltaic cell. The construction of photovoltaic cell includes semiconductor components arsenide, indium, cadmium, silicon, selenium, and gallium are utilized to create PV cells. The main materials utilized to create the cell are silicon and selenium. The most used semiconductor material for making solar cells is silicon. There are four valence electrons in the silicon atom. Each silicon atom in a solid crystal exchanges one of its four valence electrons with the next-closest silicon atom, forming covalent bonds between the two (Siva Ramkumar et al., 2022). This results in a tetrahedral lattice arrangement for the silicon crystal. A portion of the light that reaches any substance is reflected, a piece is transmitted through the medium, and the remaining component is absorbed by the material.

The diagram below illustrates silicon photovoltaic cell structures. To allow light to readily penetrate the material, the upper surface of the cell is covered with a thin coating of p-type material. P-type and n-type materials, which serve as their positive and negative output terminals, are encircled by metal rings.

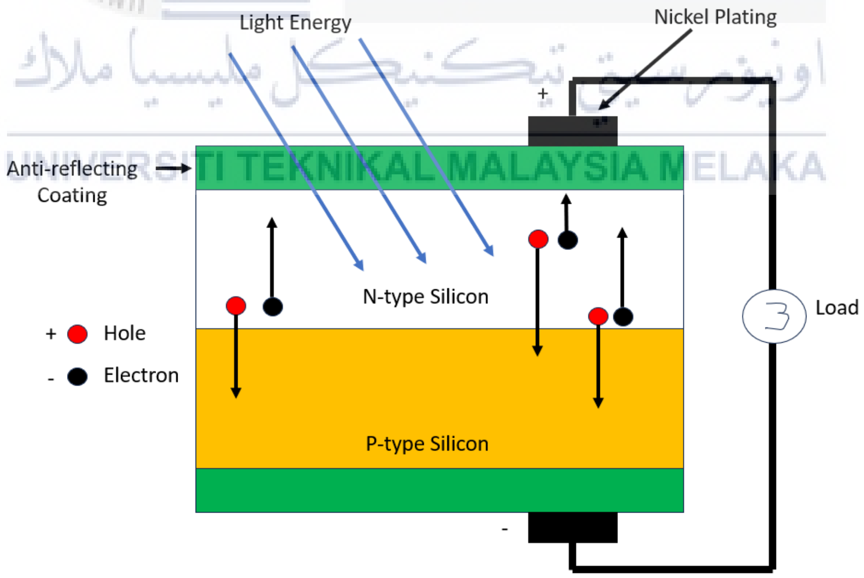

Figure 1.1: Photovoltaic cell structures with a thin coating of P-type and n-type materials

Perovskite solar cells (PSCs) were discovered as a possible choice for the upcoming generation of solar cells because of their excellent performance and low cost. The selection of the hole transport layer (HTL), which oversees improving the movement of positive charges from the perovskite layer to the electrode, has an impact on the performance of PSCs. Graphene oxide (GO) has drawn a lot of interest in this context as studies have concentrated on investigating different materials as HTLs to enhance the performance of PSCs. This research demonstrates introducing GO as an HTL to PSCs which potentially enhance effectiveness by removing positive charges and lowering recombination losses. Analysis of the performance on PSCs with GO as the HTL is carried out in order to investigate the efficiency of PSCs with varying concentrations of GO and analyze its influence on the device's performance. Numerical simulations were conducted to understand the underlying mechanism involved in the performance enhancement of GO-based PSCs. The study suggests that incorporating GO as an HTL in PSCs possibly boost their performance and improve the power conversion efficiency. The results of the study applicable in the development of next-generation PSC technologies.

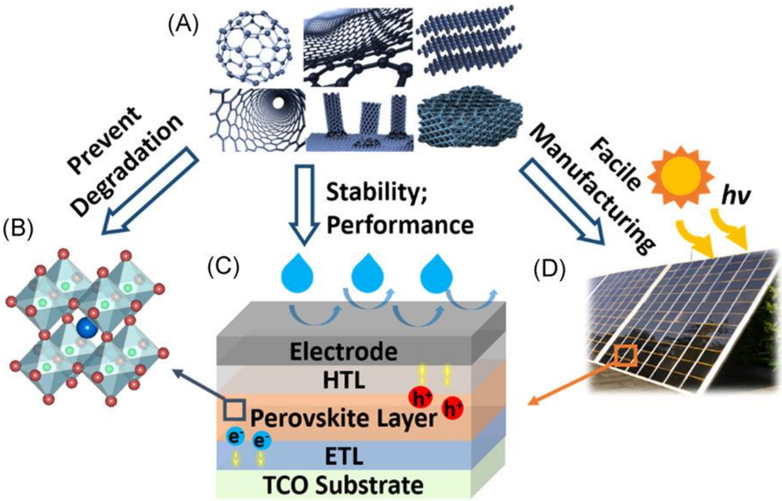

Figure 1.2: Perovskite solar cell structures

1.2 Problem Statement

Spiro-OMeTAD was primary used as the Hole Transport Material to establish high efficiency in Conventional perovskite structure. However, Spiro-OMeTAD requires equivalent dopants and substances which eventually turned out to be one of the reasons of Perovskite Solar Cells instability(Widianto et al., 2021). Alternative Hole Transport Material for Perovskite Solar Cells must be developed because of this instability and the greater costs of spiro-OMeTAD(Shariatinia, 2020)-(Nakka et al., 2022). An effective Hole Transport Material must be chemically stable, have a strong electrical conductivity, and have an energy level that matches the perovskite material. As a result, introducing Graphene Oxide (GO) as an Hole Transport Material that is both affordable and has a solid Hole Transport Layer interface is essential to achieve great Perovskite Solar Cells performance.

1.3 Research Question

The research question describe the specific subject and problem that will be the focus on this research task. It also describes the objective that to be accomplish.

i) How to simulate the thin layer Graphene Oxide as Hole Transport Material (HTM)?

ii) Why thin layer Graphene Oxide (GO) as Hole Transport Material (HTM) affect the Power Conversion Efficiency (PCE) of the perovskite solar cell?

1.4 Research Objective

The key objective of this study is to present an established and achievable methodology for developing thin layer of Graphene Oxide (GO) on Hole transport Material (HTM) for Perovskite Solar Cell. The following are the a set of objectives;

i) To simulate the thin layer Graphene Oxide as Hole Transport Material (HTM) in perovskite solar cell using SCAPs simulator.

ii) To analyse the performance of thin layer Graphene Oxide (GO) as Hole Transport Material (HTM) for perovskite solar cell.

1.5 Scope of Research

The scope of this project is to simulate thin layer Graphene Oxide as Hole Transport Material and analyze the performace of the perovskite solar cell using SCAPS-1D simulation software. There several key parameters will be optimized in order to achieve a better performance of the perovskite solar cell. The scope of this research are as follows:

- Simulate on the low-cost perovskite solar cell with thin layer Graphene Oxide as Hole.
- Optimization on several key parameter including layer thickness, acceptor density, band gaps, temperature dependence, interface defect density, resistance of Graphene Oxide (GO) as Hole Transport Material (HTM) for perovskite solar cell to achieve great performance and minimize costing.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

2.1.1 Generation of Solar cells

In recent years, the demand for renewable energy resources has been increasing rapidly due to concerns about climate change and the depletion of traditional energy resources. Solar cells, also known as photovoltaic cells, are a promising technology for renewable energy generation. Solar cells convert sunlight directly into electricity, eliminating the need for fuel, emissions, and other pollutants. The technology has evolved significantly over the years, with improvements in efficiency, design, and manufacturing, making it an increasingly viable option for large-scale energy production and smaller applications(Ranabhat et al., 2016).

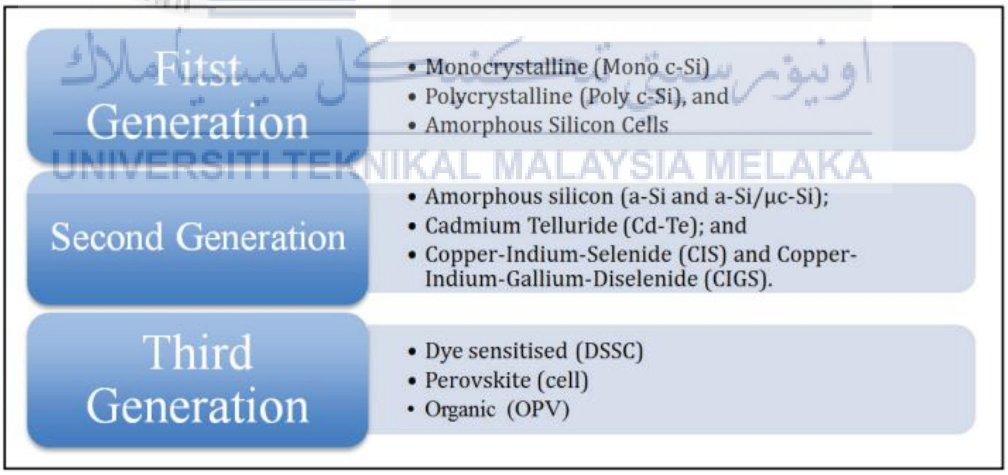

Figure 2.1: Classification of solar cells Generation

Bell Laboratories created the first generation of a solar cell with a 6% efficiency in 1954. The first commercial silicon was conventional silicon-based solar cells. They are among the finest efficient solar cells obtainable for household use, accounting for over 80% of all solar panels manufactured globally. The semiconductor material best suited for photovoltaic applications are silicon solar cells which have an energy band gap of 1.1 eV. Depending on the method the Si wafers are manufactured, the crystalline silicon cells are categorized into three major types. Monocrystalline (mono-Si), Polycrystalline (poly-Si), and Amorphous Silicone cells are available, depending on the type of silicone used. The solar cells in this generation are composed of thin silicon wafers and are referred to as monocrystalline solar cells since they are manufactured from huge single crystals.

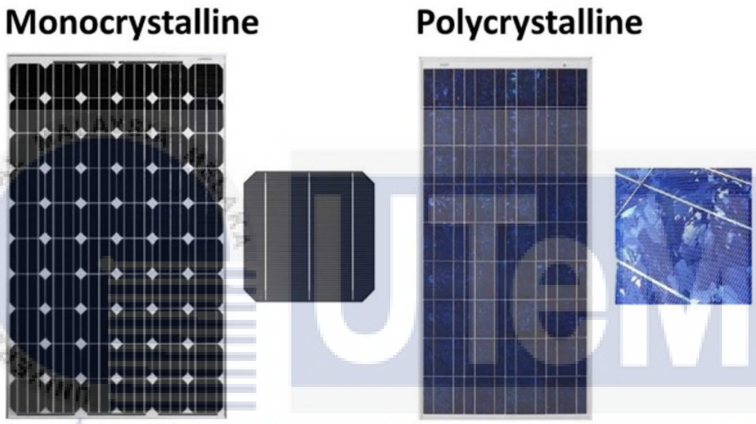

Figure 2.2: Polycrystalline and monocrystalline solar cell

As opposed to silicon-based crystalline cells, second-generation solar cells are referred to as thin-film solar cells since their layers are only a few micrometers thick. Amorphous silicon (a-Si), Cadmium Telluride (CdTe), Copper Indium Selenide (CIS), and Copper Indium Gallium Di-selenide (CIGS) are the three fundamental types of economically developed thin film solar cells. The costs and effectiveness of the second generation are lesser than those of the first generation. Thin-film solar cells are considerably more suitable for integration into walls, cars, buildings, and other surfaces because they don't require metallization on the fingers in front of them.

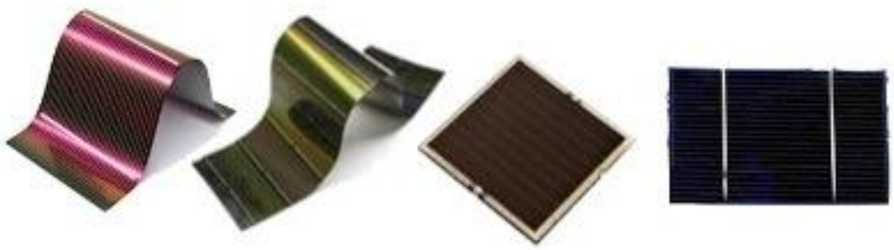

Figure 2.3: Types of Copper Indium Gallium Selenide and Copper Indium Diselenide (CIGS/CIS) solar cell

Meanwhile, third generation solar cell technologies with second generation thin-film manufacturing techniques are anticipated to generate high-efficiency devices. As a result of the costly nature of first-generation solar cells, as well as the contaminants and limited availability of ingredients for second-generation solar cells, a third generation of solar cells has emerged. They may also rely on environmentally conscious and accessible materials. These third-generation technology would also be consistent with widespread photovoltaic deployments. The strategy differs from the first generation's production of outstanding-quality, low-defect single-crystal solar energy generation systems that have high performances that exceed the limitation performances for single bandgap devices but employ energy-intensive processes.

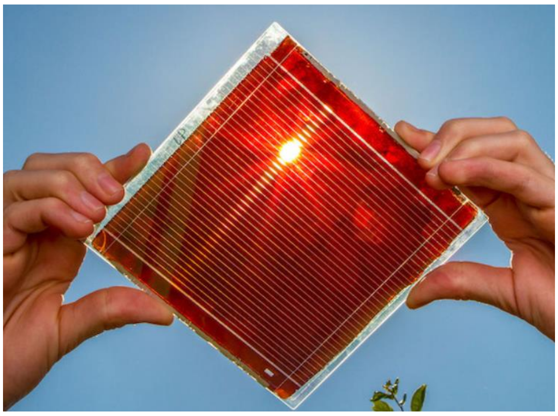

Figure 2.4: Perovskite Solar Cell