ANALYSIS OF INVERTED PLANAR PEROVSKITE SOLAR CELLS WITH GRAPHENE OXIDE AS HTL USING TAGUCHI METHOD.

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2022/2023

DECLARATION

I declare that this report entitled "ANALYSIS OF INVERTED PLANAR PEROVSKITE SOLAR CELLS WITH GO AS HTL USING L9 OA TAGUCHI METHOD" is the result of my own work except for quotes as cited in the references.



Date : 13 JANUARI 2023

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



DEDICATION

First and foremost, I am very grateful to all the family members for their valuable guidance and support in the completion of this project in its entirety. I would like to express our deepest appreciation to all those who provided us the possibility to complete our Integrated Design Project. A special gratitude I give to my supervisor, PM. Dr. Fauziyah Binti Salehuddin and co supervisor Ts. Dr. Faiz Bin Arith whose contribution in stimulating suggestions and encouragement and help me a lot in this project and with much appreciation too because she and he gave the knowledge about this project to use all required equipment and the necessary materials to complete the project. Besides, not to forget our coordinator of this PSM Project, Dr. Mas Haslinda who keep reminding us about the important things that must be implemented before the due date and always give us moral support to complete our project. Next, I also appreciate the guidance given by panels that have improved our project and the knowledge that gives us the idea to complete this project. Finally, gratitude goes to all my friends who directly or indirectly helped me to complete this project

ABSTRACT

This project studies optimization of graphene oxide (GO) as hole transport layer (HTL) in inverted perovskite solar cells (IPSC) using Taguchi method. This method is used to optimize the data from numerical modelling which is Solar Cell Capacitance Simulator-One Dimensional (SCAPS-1D). While it has variations parameters result and different factors it also requires a lot of time consuming to implement an analysis process. Taguchi method was reported can find the most prominent factor and reduce variations parameters. The Taguchi algorithm is implemented in this experiment because it is based on orthogonal array (OA) experiments, which provides substantially lower variance for the experiment with optimal control parameter values. SCAPS-1D are used to simulate the IPSC with GO as HTL. The result obtained from the software are then analyzed and compared the performance of the solar cell. Analyze the IPSC with GO as HTL with parameter power conversion efficiency (PCE), fill factor (FF) and achieve optimum performance with open circuit voltage (V_{0C}) and a density of current short circuit (J_{SC}), all of which have substantial effects on the performance of the PSCs device.

ABSTRAK

Projek ini mengkaji pengoptimuman graphene oxide (GO) sebagai lapisan pengangkutan lubang (HTL) dalam sel solar perovskite terbalik (IPSC) menggunakan kaedah Taguchi. Kaedah ini digunakan untuk mengoptimumkan data daripada pemodelan berangka iaitu Solar Cell Capacitance Simulator-One Dimensional (SCAPS-1D). Walaupun ia mempunyai hasil parameter variasi dan faktor yang berbeza, ia juga memerlukan banyak masa untuk melakukan proses analisis. Kaedah Taguchi dilaporkan boleh mencari faktor yang paling menonjol dan mengurangkan parameter variasi. Algoritma Taguchi dilaksanakan dalam eksperimen ini kerana ia berdasarkan eksperimen tatasusunan ortogon (OA), yang memberikan varians yang jauh lebih rendah untuk eksperimen dengan nilai parameter kawalan optimum. SCAPS-1D digunakan untuk mensimulasikan IPSC dengan GO sebagai HTL. Hasil yang diperoleh daripada perisian kemudiannya dianalisis dan dibandingkan prestasi sel suria. Analisis IPSC dengan GO sebagai HTL dengan kecekapan penukaran kuasa parameter (PCE), faktor isian (FF) dan capai prestasi optimum dengan VOC dan, JSC yang kesemuanya mempunyai kesan yang besar pada prestasi peranti PSC.

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LIST OF SYMBOLS AND ABBREVIATIONS

HTL	:	Hole Transport Layer
ETL	:	Electron Transport Layer
GO	:	Graphene Oxide
r GO	:	Reduce Graphene Oxide
PSC	in star	Perovskite Solar Cell
IPSC		Inverted Perovskites Solar Cell
SCAPS		Solar Cell Capacitance Simulator
PCE	100	Power Conversion Efficiency
FF	K	اونيوبرسيتي تيڪنيڪل مFill Factor
V _{oc}	iniv	Open Circuit Voltage
J _{sc}	:	Density of Short Circuit Current
OPV	:	Organic Perovskites
OA	:	Orthogonal Array
ITO	:	Indium Tin Oxide
FTO	:	Fluoride Tin Ox
Ag	:	Silver

CHAPTER 1

INTRODUCTION



This chapter describes the idea of the GO as an HTL in the solar cell which includes the background of the project, problem statement, objectives, and scope of the project.

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1.1 Background of project

The sun is a renewable resource that has the ability to sustain life on earth by providing clean, renewable energy to all of its inhabitants. Nowadays, renewable energy is the fastest-growing energy source worldwide because it is sustainable and does not produce pollution to the environment. It is projected that the current share of renewable energy sources in global energy consumption surpasses 20 % and continues to rise. Renewable energy sources, as ecologically beneficial energy resources, will become even more significant in the future because it limitless and influence the

additional energy forms in addition to the conventional power plants that are already in use [1].

The common source of renewable energy used worldwide is solar energy. It is a renewable energy source capable of providing sufficient power to households. Solar energy is an inexhaustible source of renewable energy derived from the sun's electromagnetic radiation. It generates electricity and heat fully sustainably and at no expense. Solar energy does not contribute to global warming or air pollution. The sun emits energy in the form of solar radiation, which is converted into usable energy by technology such as solar cells, also known as photovoltaic or PV cells.

Solar PV technology is a viable technique to collect solar energy since it creates electricity directly from solar radiation on-site through the photovoltaic effect of solar cells [2]. When a PV cell is exposed to sunlight, solar energy is transformed into electricity by the photovoltaic effect. Photovoltaic effect plays a key role in producing electricity from solar radiation.

Perovskite has the outstanding capabilities for use as light harvesters in solar cells

due to the ability to adjust its optical properties. Perovskite materials can be used not only as a light-absorbing layer but also as an electron/hole transport layer due to its high extinction coefficient, high charge mobility, long carrier lifespan, and long carrier diffusion distance [3]. It also acts as a charge carrying material. Perovskite solar cells have two structure which is n-i-p (regular) and p-i-n (inverted). The different between these two structures is the position of HTL and ETL. For the perovskite solar cells with inverted structure (IPSC) the HTL layer place on top of TCO (transparent conducting oxide) substrate while perovskite solar cells with regular structure (PSC) the HTL layer place between metal and perovskite substrate.



Figure 1.1: Inverted and Regular Planar Structure of Perovskite Solar Cells

The ETL and HTL layers offers a driving force for the carrier transport. These two layers may also provide protection of the perovskite layer from moisture and metal diffusion from connection. Both of it can reduce the cell's PV performance. After that, TCO substrate is needed for perovskite solar cells. It should have excellent transmission, conductivity, and adherence to the deposited layers.

The object of the Taguchi method is to identify the most significant components in a manufacturing process for accomplishing beneficial goals. These parameters are systematically modified across two or more tiers. To demonstrate the effects of each probable primary factor, the tests are designed in accordance with an orthogonal array. Orthogonal Array (OA) is one of the most significant advantages of the Taguchi method. Taguchi method also helps in minimizing the number of experiments required in optimization purpose [4].

1.2 Problem Statement

The important characteristics of HTL is high conductivity, high transparency, favorable solution processability and stability, high WF and good hole mobility [5]. In this experiment, IPSC devices can improve the stability of solar cell compared to

Planar Perovskite Solar Cells (PSC) [6]. Next, OPV cells have a substantially lower efficiency than inorganic-based devices, which is a major flaw at the moment. Organic semiconductors have a bigger band gap than inorganic semiconductors. Nevertheless, OPV use Spiro-OMeTAD which is dopants in that material show strong water absorbency, stability issues arising from photochemical degradation (exposure to moisture or humidity) which seriously threatens the service life of PSCs. The costs of organic materials such as spiro-OMeTAD, PEDOT:PSS, PTAA and P3HT are all prohibitively high for large-scale applications [7]. The industrial growth and market potential of photovoltaic solar cells (PSCs) is constrained by their high cost and instability in water, heat, and light, despite the fact that all of these materials provide higher open-circuit voltages and higher efficiencies. [8].

1.3 **Objective**

Specifically, the objectives of the project are:

(i) To simulate the inverted Planar Perovskite Solar Cells (IPSC) with GO as HTL using SCAPS-1D software.

(ii) To analyze the parameters such as power conversion efficiency (PCE), fill factor (FF), density of short-circuit current (J_{sc}) and open-circuit voltage (V_{oc}).

(iii)To optimize the GO layer as HTL of the IPSC using Taguchi Method.

1.4 Scope of work

This project is to analyze GO as HTL layer on the emerging solar cell which is IPSC. The analysis is conducted by simulation method using SCAPS-1D software. After simulation, analyzed from I-V curve the power conversion efficiency (PCE), fill factor (FF) and achieve optimum performance with open circuit voltage (V_{oc}) and a

density of current short circuit (J_{SC}). The efficiency of the solar cells will be optimized by controlling several parameters of the HTL. The parameters included are the HTL thickness, doping density, working temperature, and defect density [8]. To achieve maximum efficiency, those parameters of each layer of the solar cell were researched thoroughly. Taguchi Method is a process for optimizing a number of control parameters that directly determine the target or desired output value. The optimization process then entails establishing the optimal control factor levels to obtain the desired outcome.

1.5 Thesis outline

This thesis consists of five chapters and those are introduction, literature review, methodology, results, and discussion and finally conclusion and recommendation. Each section explains in detail with the depth of this project. The introduction of this project is explained in Chapter 1. In this section explanation of the background, objectives of the project, problem statement, project scope and thesis outline are listed with details.

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The literature review is described in Chapter 2. The project's research was reviewed in order to compile all key information. In addition, a few initiatives identical to this thesis were researched to ensure a positive outcome. This project's methodology is described in the Chapter 3. This chapter will cover the project activities, which includes the entire design using SCAP-1D software and optimize using L9 OA Taguchi Method. This chapter will go through each simulation design in detail.

The results and discussion from this project's simulation are described in Chapter 4. This chapter will explain the results obtained and also analyzed and discussed the results. To obtain a better efficiency, the optimum value based on optimization using Taguchi method need to be obtained. The efficiency of IPSC with GO as HTL can be determined and compare before and after optimization. The project's conclusion and recommendations are described in Chapter 5. The entire project and the achievement of project objectives are concluded in this section. The recommendation is to conduct further study in order to improve the situation.



CHAPTER 2

BACKGROUND STUDY

This chapter provides an overview of theoretical frameworks which includes the previous research on GO and other HTL materials.

2.1 Inverted Perovskite Solar Cells (IPSC)

Perovskite solar cells have experienced a rapid development and shown great **UNVERSITITEKNIKAL MALAYSIA MELAKA** potential as the next-generation photovoltaics. For the inverted perovskite solar cells PSCs, the device efficiency has reached a power conversion efficiency (PCE) 23.7%. According to the M. Degani et al., (2021) inverted perovskite solar cells use a novel technique to optimize the interfaces by promoting high-quality film formation on top of the HTL and inducing effective defect passivation at the perovskite interface. This improvement can increase in the fill factor (FF) accompanied by a small increase in the short circuit current (J_{sc}) and open circuit voltage (V_{oc}). Hence, the inverted perovskite solar cells have a high PCE and low hysteresis. The efficiency of IPSC more than 21% which is comparable to the highest performing regular type PSCs [9].



Figure 2.1: Inverted Perovskite Solar Cells Structure

2.1.1 Hole Transport Layer

Hole transport material is an important component in Inverted Perovskite Solar Cell (IPSC). It has the function of adjusting the energy compatibility, optimize the interface and to gain higher PCE. The hole transport layers can be divided into three categories, which are organic HTL, Polymeric HTL and inorganic HTL. Only the first and third category will be discussed in this sub chapter.

HTL is inorganic p-type due to higher mobility, chemical stability and increased transparency in the visible region [10]. Due to its good transparency, it will significantly increase the efficiency [11]. According to Salim et al., (2015) The transportation layers utilized in the device architecture determine the stability and performance because it serve numerous features in PSCs such as; (i) it acts as energetic barrier between ETL and perovskite layer by blocking the electron transfer; (ii) when efficiency of HTL improves due to its high mobility and its matching energy level with those of ETLs/HTLs and electrode; (iii) avoids the deterioration and corrosion that can occur at the metal-perovskite interface without an HTL [12].

According to several research results, inorganic materials that usually used as HTL are CuSCN, NiOx, CuO and GOx. An example, Nickel oxide (NiOx) as HTL with

expected stability as it has good optical transparency, prevents electron leakage and has appropriate energy levels. An excellent HTL must have the optimum energy level for the perovskite material, as well as high electrical conductivity, optical transparency, and chemical stability [12],[13].

NO.	Class Material Base	V _{oc}	J _{sc}	FF (%)	PCE	Year	Ref.
	HTL	(V)	$(mAcm^{-2})$		(%)		
1	Carbon, GO,	0.93	21.71	81.49	16.51	2021	[14]
	CH ₃ NH ₃ PbI ₃ , TiO ₂ ,						
	FTO						
2	ITO, GO,	0.94	20.00	78.7	14.70	2019	[15]
	Cdot						
	MAPbI ₃ , PCBM,						
	BCP						
3	ITO, ZnO,	0.62	13.00	51.14	4.13	2022	[16]
	PC ₆₀ BM, P3HT, PH5						
	GO1, PH5						
4	Al, LiF, P3HT:	0.53	14.00	38	2.80	2018	[3]
	PCBM, PEDOT:						
	PSS-GO, ITO	1/	./ .				
5	Ag, GO,	1.04	24.44	73.12	18.53	2021	[17]
	TiO_2 , $CH_3NH_3PbI_3$,	-		V	1.		
	FTOJIVERSITI T	EKNIK	AL MALA	YSIA ME	LAKA		
6	ITO, PEDOT: PSS,	0.55	9.71	36.4	4.02	2021	[18]
	GOAg, P3HT:						
	PCBM, Ca, Al						
7	FTO, c-TiO ₂ , mp-	0.93	17.67	70	11.50	2021	[19]
	TiO2, rGO:						
	MAPBI3, Ag						
8	Ag, ETL,	1.05	22.17	76.78	17.84	2019	[20]
	$CH_3NH_3PbI_3$,						
	NiOx, ITO						

Table 2.1: The Parameters of PSC with Different Class of HTLs

The J_{SC} can be defined in the Shockley equation, and it can be described as Equation (2.1) [21]:

$$J_{SC} = J_o \left[exp\left(\frac{q(V-JRs)}{nkT}\right) - 1 \right] + \frac{V-JRs}{R_{SH}} - J_{Ph}$$
(2.1)

Where;

 J_{Ph} = Photocurrent density

 J_o = The dark saturation current

k = Boltzman Constant

T = Room Temperature

q = Electronic Charge

In an ideal condition, RS must be zero, and RSH should be infinite. J_0 and J_{sc} was depends on V_{OC} . This equation was formulateed from Green and Cells in 1982 [22]. The Equantion (2.2) as shown:



 $I_{SC} = Short Circuit current (A)$

 $V_{OC} = Open Circuit voltage (V)$

PCE
$$(\eta) = \frac{V_{OC} \times I_{SC} \times FF}{P_{in}} \times 100\%$$
 (2.4)

All these inorganic materials of HTL are used in order to replace organic HTLs. By using inorganic semiconductor materials, a good efficiency can be obtained different with organic perovskite solar cells (OPV). Herewith some of the recent reviews from Rajeswari et al. (2017) have been analyzed and discussed about the efficiency and stability of PSCs have been researched. However, the efficiency of OPV cells is much lower than that of inorganic-based devices. Organic semiconductors have a significantly larger band gap, are unstable in water, heat, and light. [23] and the costs of spiro-OMeTAD, PEDOT: PSS, PTAA and P3HT are all prohibitively high for large-scale applications [7]. The standard organic perovskite cells normally use PEDOT: PSS and Spiro-OMeTAD as the HTL.

2.1.1.1 Graphene Oxide (GO)

Graphene has a hexagonal structure and composes of sp2hybridized carbon atoms. From previous research, GO is known as an excellent interfacial material [13]. GO has sparked a lot of interest due to its remarkable characteristics, reliability, low processing cost, large-scale production possibilities, and good dispersibility in a variety of solvents [14]. Due to its high charge mobility, the GO can provide energy compatibility by providing a sufficient exciton breakup the path and charge transport with the photoactive layer, either as transparent conductive electrodes, ETL, or HTL [24]. According to Cho et al., (2014) GO and r-GO, which have a two-dimensional sheet structure consisting of carbon atom monolayers, are considered to have a high potential for use in PSCs when compared to carbon materials because it have good electrical conductivity and a large specific surface area [25].

Graphene derivatives GO and r-GO have thus been used as a substitute for spiro-OMeTAD as HTL in PSCs due to the aforementioned features. Due to the device's mobility and stability, this could be a viable solution both economically and technically [16]. Replacing organic HTL with GO could improve efficiency, and r-GO could be a viable candidate for boosting cell stability. From research journal PEDOT: PSS/GO blend as an HTL on top of a hydrophobic photoactive layer. Pure PEDOT: PSS characteristics have limits its application potential due to its highly hydrophilic nature, it has a surface energy mismatch and the conductivity range use in electrodes are very low [26]. PEDOT: PSS has been modified with GO materials possess several advantages. The advantages that are suitable for OPVs application is high surface area, conductivity, and mechanical elasticity [27]. Besides, GO wide bandgap (~3.6 eV) can enhance the potential for utilization as an electron blocking layer [28].

GO as HTL in inverted PSC shows that GO has a suitable WF of - 4.9 eV which accumulates efficient hole extractions from perovskite to GO. Extractions from perovskite to GO; thus, forming homogeneous big domains with enhanced surface coverage and appropriate vertical resistivity is facilitated. As a result, the PCE of the PVSC with GO HTL increases [11]. This GO modified PEDOT: PSS maintained 83.5% of its initial PCE value, indicating that using the GO-modified PEDOT:PSS as HTL rather than the unmodified PEDOT as HTL appears to be a good strategy for enhancing the effectiveness and stability of PSCs [8].

2.1.1.2 Taguchi Method

Taguchi method is a method used to improve the quality of the analyzed processes and products. This method, which is based on a predictive model, specifically the analysis of S/N ratios, permits the control of many components in order to limit parameter changes and alter the experimental process under the same experiment circumstances, resulting in improved response analysis and physical attributes [29]. Indeed, the Taguchi method has been effectively implemented for a variety of systems and materials with a high level of complexity in a variety of scientific, engineering, and industrial fields, and it has been proven to be a reliable and reputable methodology with high reliability and product quality [30].

The Taguchi technique is used to identify the most essential aspects in accomplishing beneficial outcomes in a manufacturing process. These variables are systematically altered at two or more levels. According to H. Absike, described in this paper the development and characterization of copper oxide thin films using the Taguchi method to optimize the structural and optical properties of films formed under optimum conditions. Three parameters, namely Cu2+ content, preheating temperature TP, and final heat-treatment temperature, were chosen. [31].

The signal to noise ratio (S/N) was determined to examine the experimental data and determine the elements that influenced the response. According to Taguchi method, the best values for each chosen experience were determined by comparing the signal-to-noise (S/N) ratio in order to allow "the greater the better" response and make the device superior performance [32].

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CHAPTER 3

METHODOLOGY

This section explains how to use the data and information gathered using a certain technique to acquire and achieve the project's objectives. This section also includes the key flowchart for this concentration in order to make the task embraced clearer and methodically based in order to achieve better and better results. This part will provide an overview of the technique that will be used, which will cover the complete scope of this project.

3.1 Overview

This analysis has two part which is simulation and optimization the result using Taguchi method. The simulation part is carried out by using SCAPS-1D software where the solar structure of IPSC is simulated initially to analyze the optimum efficiency. The IPSC structure is investigated in various aspects including the working temperature, the thickness of GO or HTL, doping density and the defect density. From SCAPS-1D the I-V characteristics are used to evaluate the PCE, FF, V_{oc} and J_{sc}. Then

after collect all the data, optimize the data using Taguchi method in order to obtain the effective result.

3.2 Flowchart of the project

In this project, there are a few methods that have been carried out to obtain the desired results. All the steps involved will be explained based on the flowchart as shown in Figure 3.1.



Figure 3.1: Flowchart of the Project

3.3 Flowchart of Taguchi Method

This project utilized the Taguchi method to determine the optimal solution for IPSC devices. Taguchi method emphasizes the design and execution of experiments that can determine the effect of input process parameters on output responses. By analyzing the impact of different components, the optimal combination of factors can be identified. Figure 3.2 depicts the primary implementation processes for Taguchi method input process parameter optimization.



Figure 3.2: Flowchart of Taguchi Method

3.4 Simulation

3.4.1 SCAPS-1D

SCAPS-1D (version 3.3.10) numerical modelling simulation tool up to seven semiconductor layers developed by a photovoltaic researcher at the University of Gent's Department of Electronics and Information Systems. For solar cell devices with up to seven semiconductor layers, SCAPS-1D extracts the electrical parameters such as acceptor and donor density, current densities and so on. Solving the Poisson equation in Equation (3.1) and the continuity equations for electrons and holes in Equations (3.2) and (3.3) respectively. These equations contained in the programmed provides the spectrum response of solar radiation and current-voltage (J-V) characteristics [14].

$$\frac{d}{dx} \left[\epsilon(x) \frac{d\Psi}{dx} \right] = q \left[p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x) \right]$$
(3.1)

$$\frac{1}{q}\frac{dJ_n}{dx} + R_n(x) - G(x) = 0$$
(3.2)

(3.3)
$$\frac{dJ_p}{dx} + R_p(x) - G(x) = 0$$

Where, Ψ = electrostatic potential, ε = dielectric permittivity (relative), x = denotes the position, N_A^- = ionized acceptor, N_D^+ = ionized donor, p = holes, e = electrons, p_t = number of trapped holes, n_t = number of trapped electrons, J_p = holes current density, J_n = electrons current density, G(x) = generation rates, $R_p(x)$ = recombination rate of holes and $R_n(x)$ = recombination rate of electrons. It allows the user to model the bandgap energy diagram and the I-V curve of a solar cell by constructing a p-n junction, adding contacts, and simulating the bandgap energy diagram and I-V curve. SCAPS is a simple application that may be used for both research and education. Meanwhile, Figure 3.3 shows the working point and lighting are set on the action panel of SCAPS. In SCAPS-1D the set problem is used to design each layer of solar cell structure, to insert electrical parameter, and add interfaces between layers. The action setting is used to show the client which estimation of the sun-powered cell to reproduce. I-V quality scale adjustment, C-V capacitance voltage adjustment, C-f capacitance recurrence adjustment, and QE quantum productivity adjustment are all included. In this experiment, only the I-V configuration will be used to determine the Power Conversion Efficiency (PCE). The solar cell's scope, which is somewhere between V1 and V2, has been set to 0 V and 2 V, respectively. For the diagram and boundary of the solar cell to be shown after executing the application, this reach needs be set at a specific value. The illumination setting is used to set the range and the course of the prevailing light condition, which can be dull or bright. The daylight was adjusted to a standard brightness of AM1.5G, 100mWcm² and the light in the enlightenment setting was turned on. Before calculating single shot need to set the temperature of the sunlight intensity. The temperature can set in kelvin unit.

						1 1	
SCAPS 3.3.10 Action Par	nel					-	- 🗆 ×
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Illumination: Dark Lig	ht Specify	/ illumination spe	ctrum, then calcu	late G(x)	Directly specify G	(x)	
Analytical model for spectrum Spectrum file name: illumin: Select spectrum file Spectrum cut off ?	Amilia Spectrum from file ated from left illumina AM1_50 Short wavel. (nm) 200 Long wavel. (nm) 400	ted from right G 1 sun.spe .0	c Inciden light powe sun or lamp 10 after cut-off 10	t (or bias) er (W/m2) 00.00	Analytical moo G(x) model Ideal Light Cur Transmission o	Constant gene rent in G(x) (mA, f attenuation filte	G(x) from file ration G /cm2) 20.0000 er (%) ■ 100.00
Neutral Density 🖨 0.0000	Transmission (%) 韋 100	.000	after ND 10	00.00	ldeal Light Cu	rrent in cell (mA)	/cm2) 0.0000
Action	se at each step						
	V1 (V) 🖨 0.0000	V2 (V) 🖨	b) ₀₀	🔽 Stop after	Voc 101	\$ 0.0200	increment (V)
r≕ -v r≕ c-v	V1 (V) ♦ 0.0000 V1 (V) ♦ -0.8000	V2 (V) 🜲 V2 (V) 🖨	<mark>b)</mark> 00 0.8000	🔽 Stop after	voc € 101 € 81	0.02000.0200	increment (V) increment (V)
□V □ C-V □ C-f	V1 (V)	V2 (V) ↓ V2 (V) ↓ f2 (Hz) ↓	D) 00 0.8000 1.000E+6	🔽 Stop after	v Voc ↓ 101 ♣ 81 ♣ 21	 0.0200 0.0200 5 	increment (V) increment (V) points per decade
□ FV □ C-V □ C-1 □ QE (IPCE)	V1 (V) ♥ 0.0000 V1 (V) ♥ -0.8000 f1 (Hz) ♥ 1.000E+2 WL1 (nn) ♥ 300.00	V2 (V) ↓ V2 (V) ↓ f2 (Hz) ↓ WL2 (nm) ↓	D) ₀₀ 0.8000 1.000E+6 900.00	☑ Stop after	voc \$101 \$81 \$21 \$61	 0.0200 0.0200 5 10.00 	increment (V) increment (V) points per decade increment (nm)
FV C-V C-f Cf Cf Set problem	V1 (V) € 0.0000 V1 (V) € 0.8000 f1 (Hz) € 1.000E+2 WL1 (nm) € 300.00 Ioaded definition file:	V2 (V) ↓ V2 (V) ↓ f2 (Hz) ↓ WL2 (nm) ↓	D) ₀₀ 0.8000 1.000E+6 900.00	Stop after	Voc 101 31 31 31 31 31 31 31 31 31 3		increment (V) increment (V) points per decade increment (nm) em
 FV C-V C-f QE (IPCE) Set problem Calculate: single shot	V1 (V) € 0.0000 V1 (V) € 0.8000 f1 (Hz) € 1.000E+2 WL1 (nm) € 300.00 loaded definition file: Continue	V2 (V) ♣ V2 (V) ♣ f2 (Hz) ♣ WL2 (nm) ♣	b) ₀₀ 0.8000 1.000E+6 900.00 a) Resu	Violation Stop after Protection P	Voc 101 81 21 61 blem file: new proble ations		increment (V) increment (V) points per decade increment (nm) em ve all simulations
FV FV C·V C·f C·f OE (IPCE) Set problem Calculate: single shot Calculate: batch	V1 (V) € 0.0000 V1 (V) € 0.8000 f1 (Hz) € 1.000E+2 WL1 (nm) € 300.00 loaded definition file: Continue Batch set up	V2 (V) € V2 (V) € f2 (Hz) € WL2 (nm) €	b) ₀₀ 0.8000 1.000E+6 900.00 a) Resu	Stop after Pro	vVoc ♥ 101 ♥ 81 ♥ 21 ♥ 61 Diem file: new proble ations C-V C-f Qi		increment (V) increment (V) points per decade increment (nm) em ve all simulations ar all simulations
FV C-V C-f C-f Cef OE (IPCE) Set problem Calculate: single shot Calculate: batch Calculate: recorder	V1 (V)	V2(V) € V2(V) € 12(Hz) € WL2(nm) € Stop	b) ₀₀ 0.8000 1.000E+6 900.00 a) Result (, , , , , , , , , , , , , , , , , , ,	From Prove Its of calcul C I-V (ecorder rest	PVoc 0 points € Voc 0 101 € 81 € 21 € 61 € 61 Elem file: new proble ations C-V C-f QI ults		increment (V) increment (V) points per decade increment (nm) em ve all simulations ar all simulations SCAPS info
FV C·V C·V C·f OE (PCE) Set problem Calculate: single shot Calculate: batch Calculate: recorder Calculate: recorder Calculate: curve fitting	V1 (V) € 0.0000 V1 (V) € 0.8000 f1 (Hz) € 1.000E+2 WL1 (nm) € 300.00 Ioaded definition file: Continue Batch set-up Record set-up Curve fit set-up	V2 (V) € V2 (V) € I2 (Hz) € WL2 (nm) € Stop	b) ₀₀ 0.8000 1.000E+6 900.00 2) Rest G,R) A R Cu	Stop after Pro Its of calcul C [1-V] corder rest rvefitting res rvefitting res rest rvefitting res rvefitting res rest res rest rest rest rest rest rest	vvcc 0 points 101 € 81 € 21 € 61 Diem file: new proble ations C-V C-f Qt ults sults		increment (V) increment (V) points per decade increment (nm) em ve all simulations ar all simulations SCAPS info

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Figure 3.3: SCAPS-1D Action Panel

3.4.2 SCAPS-1D problem setting

Figure 3.4 shows the SCAPS-1D software and it consists of four settings. After clicking on set problem, as shown in Figure 3.4, the solar cell defining board is opened. There are three classifications on this board. There are five buttons on it. These buttons have the ability to create new, load, and save construction records in the SCAPS definition library. The layers of the solar cell are saved as '.def' files. After characterizing the design, the 'ok' button is pressed.



Figure 3.4: SCAPS-1D Solar Cell Definition Panel

3.4.3 SCAPS-1D adding layers to structure

As show in Figure 3.5, the setting layer, it consists of interface between layer, back and front contact and mathematical inclinations. The SCAPS-1D can only assist in the creation of a sun-powered cell with up to 7 layers. In this segment it can change the position of illuminated from left or right. A few buttons are used to applied voltage and current. It also can see the thickness and the color each layer of solar cell. In this SCAPS-1D layer properties board are used to insert the electrical parameter each of the material. The mathematical examination boundaries for each layer in IPSC devices are based on the SCAPS –ID input parameter from previous researchers as shown in Table 3.1.

thickness (µm) C 10 The layer is pure A: y = 0, uniform 000 Semiconductor Property P of the pure material 000 Semiconductor Property P of the pure material 000 bandgap (eV) 233 dielectron affinity (eV) 233 dielectron affinity (relative) 100 C 8 effective density of states (1/cm ² 3) 242 V 8 effective density of states (1/cm ² 3) 138 electron thermal velocity (cm/s) 520 hole thermal velocity (cm/s) 521 hole thermal velocity (cm/s) 520 hole themobility (cm/Vs) 246 hole mobility (cm/Vs) 122 Allow Tunneling effective mass of holes 100 no ND grading (uniform)	100		
Uninf Uninf The layer is pure A: y = 0, uniform 0.00 Semiconductor Property P of the pure material pur bandgap (eV) 24 electron affinity (eV) 23 dialectric permittivity (relative) 100 CB effective density of states (1/cm ⁻³) 22 be effective density of states (1/cm ⁻³) 23 be effective density of states (1/cm ⁻³) 25 hole thermal velocity (cm/s) 5.00 belectron mobility (cm/Vs) 2.66 hole mobility (cm/Vs) 2.66 hole mobility (cm/Vs) 2.61 hole mobility (cm/Vs) 12 Allow Tunneling effective mass of electrons 100 on ND grading (uniform) 100		Band to band recombination	
The layer is pure A: y = 0, uniform 0.00 Semiconductor Property P of the pure material pur bandgap (eV) 244 electron affinity (eV) 233 dielectric permittivity (relative) 101 CB effective density of states (1/cm ³) 224 be effective density of states (1/cm ³) 218 electron hermal velocity (cm/s) 520 hole hermal velocity (cm/s) 522 hole mobility (cm?/vs) 266 hole mobility (cm?/vs) 266 hole mobility (cm?/vs) 12 Allow Tunneling effective mass of electrons 100 offective and store (100) effective mass of holes 100 no ND grading (uniform) 200 200	niform pure A (v=0)	Radiative recombination coefficient (cm ^a /s)	0.000E+0
Semiconductor Property P of the pure material pure bandgap (eV) 244 electron affinity (eV) 233 electron affinity (eV) 233 electron affinity (eV) 244 electron affinity (eV) 243 electron affinity (eV) 243 electron affinity of states (1/cm^3) 242 VP effective density of states (1/cm^3) 242 VP effective density of states (1/cm^3) 243 electron thermal velocity (cm/s) 540 electron mobility (cm²/Vs) 246 electron mobility (cm²/Vs) 246 effective mass of electrons 100 effective density (cm²/Vs) 122 effective mass of electrons 100 effective mass of foles 100 no ND grading (uniform)	000	Auger electron capture coefficient (cm^6/s)	0.000E+0
bandgap (eV) 24 bandgap (eV) 23 dielectro affinity (elative) 10 bad effective density of states (1/cm^3) 18 electron thermal velocity (cm/s) 520 hole mobility (cm?Vs) 26 allow Tunneling effective mass of electrons on ND grading (uniform) 10	III = A(y = 0)	Auger hole capture coefficient (cm^6/s)	0.000E+0
bandgap (eV) 244 electon affinity (eV) 233 dielectric permitivity (relative) 100 CB effective density of states (1/cm ² 3) 221 VB effective density of states (1/cm ² 3) 181 electon thermal velocity (cm(s) 522 belecton nobility (cm ² /Vs) 500 electon nobility (cm ² /Vs) 266 hole mobility (cm ² /Vs) 12 Allow Tunneling effective mass of holes 100 no ND grading (uniform) 500 100		Recombination at defects: Summary	
electon affinity (eV) 2.3 dielectric permitivity (relative) 10.0 2.6 Bréctive density of states (1/cm²3) 2.2 VB effective density of states (1/cm²3) 1.8 electron thermal velocity (cm/s) 5.20 hole thermal velocity (cm/s) 5.00 electron nobility (cm²/Vs) 2.66 hole mobility (cm²/Vs) 1.2 Allow Tunneling effective mass of holes 1.00 no ND grading (uniform) 0.00 0.00	480		
delectric permittivity (relative) 10.1 CB effective density of states (1/cm*3) 2.2 VB effective density of states (1/cm*3) 1.8 electron nbirnal velocity (cm/s) 5.2 hole thermal velocity (cm/s) 5.2 ielectron nbirnal velocity (cm/s) 5.0 hole mobility (cm?Vs) 2.66 hole mobility (cm?Vs) 12 Allow Tunneling effective mass of electrons 10 effective mass of holes 10	300		
CB effective density of states (1/cm ⁻³) 2.21 VB effective density of states (1/cm ⁻³) 1.81 electron thermal velocity (cm/s) 5.22 hole thermal velocity (cm/s) 5.01 electron mobility (cm ² /Vs) 2.06 hole mobility (cm ² /Vs) 2.61 Allow Tunneling effective mass of electrons 1.01 no ND grading (uniform) 1.02 1.02	0.000		
VB effective density of states (1/cm^3) 18 electorn thermal velocity (cm/s) 52 hole thermal velocity (cm/s) 50 electorn mobility (cm²/Vs) 26 hole mobility (cm²/Vs) 12 Allow Tunneling effective mass of holes effective mass of holes 10 no ND grading (uniform) 10	200E+18		
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hole thermal velocity (cm/s) 5.00 electon mobility (cm?Vs) 2.60 hole mobility (cm?Vs) 1.20 Allow Tunneling effective mass of electrons 1.00 effective mass of holes 1.00 no D grading (uniform) 1.00	200E+7		
electron mobility (cm²/Vs) 260 hole mobility (cm²/Vs) 122 Allow Tunneling effective mass of electrons 100 effective mass of holes 101 no ND grading (uniform)	000E+7		
hole mobility (cm²/Vs) 12: Allow Tunneling effective mass of electrons 1.00 effective mass of holes 1.00 no ND grading (uniform)	600E+1		
Allow Tunneling effective mass of electrons 1.00 effective mass of holes 1.00 no ND grading (uniform)	230E+2		
no ND grading (uniform)	000E+0		
no ND grading (uniform)	000E+0		
shallow uniform donor density ND (1/cm3) 0.0	000E+0		
no NA grading (uniform)	-		
shallow uniform acceptor density NA (1/cm3) 2.0	000E+18		
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Set absorption model save		Defect 1	
	- 6		
List of absorption submodels present soft/hv-Eq) law (SCAPS traditional)			
		(no metastable configuration possible)	
			V /
5		Accept cancel Load M	aterial Save Material
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~		Load M	

Figure 3.5: SCAPS-1D Layer Properties Panel

#### 3.4.4 -SCAPS-1D simulation for IPSC with GO® as HTL UNIVERSITI TEKNIKAL MALAYSIA MELAKA

In this experiment, there are five layers in the IPSC device. First layer is FTO function as front contact where the metal work function for FTO is 4.4eV. Then followed by GO as the HTL, the active layer which is perovskite,  $CH_3NH_3PBI_3$ ,  $TiO_2$  as ETL and Ag as back contact where the metal work function for Ag is range from 4.26-4.73eV. There are 4 parameters have been optimized to obtain optimal effectiveness of IPSC device based on the presence of GO as HTL. The parameters are the thickness of GO, Graphene Oxide doping thickness, a deformity interface at each layer and a solar cell's operating temperature. Table 3.1 shows the numerical analysis input parameter for each component mentioned in the previous research.
Layers       Interfaces         GO       GO / Perovskite         Perovskite       GO / Perovskite         TiO2       add layer         inght contact (back)       Interfaces         Info on graded parameters only available after a calculation	×
	ture
Problem file	
c\Program Files (x86)\Scaps3309\def\ IPSC with G0 as HTL (from journal).def last saved. 77e-022 at 29.28	
Remarks (edit here)	
SCAPS 3.3.10 ELIS-UGent Version scaps3310 exe, dated 10-04-2021, 11-22-08 Problem c ⁴ new       load       savel last saved by SCAPS: 07-06-2022 at 02:09-28         Comments (to be) included in the deffile       cancel       Ot         Can be edited by the user       Ot       Ot	/e



Figure 3.7: 2D IPSC Solar cell structure

Material Properties	FTO	TiO ₂	CH ₃ NH ₃ PBI ₃	GO	
Thickness, d (um)	0.5	0.05	1	0.1	
Bandgap, Eg(ev)	3.5	3.2	1.58	2.48	
Electron affinity $\chi$ (ev)	4	4	3.9	2.3	
Dielectric permittivity, ε _r (relative)	9	9	10	10	
CB effective density of states, $N_C$ (cm ⁻³ )	$2.2 \times 10^{18}$	$2.2 \times 10^{18}$	$2.2 \times 10^{18}$	$2.2 \times 10^{18}$	
VB effective density of states, $N_V$ (cm ⁻³ )	$1.8 \times 10^{19}$	$1.8 \times 10^{19}$	$1.0 \times 10^{19}$	$1.8 \times 10^{19}$	
Electron thermal velocity $(cms^{-1})$	$1.0 \times 10^{7}$	$1.0 \times 10^{7}$	$1.0 \times 10^{7}$	$5.2 \times 10^{7}$	
Hole thermal velocity $(cms^{-1})$	$1.0 \times 10^{7}$	$1.0 \times 10^{7}$	$1.0 \times 10^{7}$	$5.0 \times 10^{7}$	
Electron mobility, $u_n$ (cm ² . V ⁻¹ s ⁻¹ )	20	20	2.2	26	
Hole mobility, $u_p$ (cm ² .V ⁻¹ s ⁻¹ )	⁵ 10	10	2.2	123	
Donor density, $N_D$ (cm ⁻³ )	$2.0 \times 10^{19}$	$2.0 \times 10^{18}$	$1.0 \times 10^{13}$	-	
Acceptor density, $N_A$ (cm ⁻³ )			$1.0 \times 10^{12}$	$2.0 \times 10^{18}$	
Defect GO/CH ₃ NH ₃ PBI ₃	12.			$1 \times 10^{10}$	
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Table 3.1: SCAPS-1D Input Parameter of Numerical for Each Layer in IPSCDevices [14]

 Table 3.2: The Parameters of the Interface Defect of HTL/Perovskite [14]

Parameters	HTL/Perovskite	ETL/Perovskite
Defect type	Neutral	Neutral
Capture cross-sections electrons	1×10 ⁻¹⁹	1×10 ⁻¹⁹
(cm ² )		
Capture cross-sections holes	1×10 ⁻¹⁹	1×10 ⁻¹⁹
(cm ² )		
Energetic distribution	Single	Single
Reference for defect energy level	Above the highest EV	Above the highest EV
Et		
Energy with respect to a reference	0.600	0.600
(eV)		
Total density $(cm^{-2})$	10 ¹⁰ (variable)	10 ¹⁰ (variable)

Parameter	Back contact (Ag)	Front contact (FTO)
Surface recombination velocity of electron (cm/s)	1×10 ⁵	1×10 ⁷
Surface recombination velocity of holes (cm/s)	1×10 ⁷	1×10 ⁵
Metal work function (eV)	4.26 - 4.73 [33]	4.3

Table 3.3: Parameter of Back and Front Contact for Ag and FTOrespectively [14]

Finally, after simulation, the I-V curve will be analyzed and see the performance of IPSC through PCE. From I-V curve it shows the  $V_{oc}$ ,  $J_{sc}$ , FF and PCE. In any case, if the results do not match the ideal result, the method should be reviewed until the ideal result is achieved.

## 3.5 **•** Method analysis

# To obtain the maximum efficiency for IPSC with GO as HTL, the important parameter value for GO as HTL and IPSC were analyzed. The parameters involved are the thickness of GO, the defect density of GO/Perovskite, the capture crosssections of holes, the capture cross-sections of electrons and working temperature of solar cell.

# 3.5.1 The effect of thickness of GO layer

One of the main factors affecting IPSC performance is the thickness of the HTL. Only the thickness of the GO layer was changed in this investigation; other component thicknesses remain constant. To begin with, a thickness range between 10 nm and 100 nm was examined to determine trends in IPSC efficiency. Then, additional analysis was performed to determine the highest solar cell efficiency that could be obtained by using GO with an ideal thickness. Additionally, the point of GO thickness where the efficiency deviates from its maximum value was noted. In this instance, the GO thickness range was determined to closely match with the reported thickness and to be consistent with previous studies.

#### 3.5.2 The effect of defect density of GO/Perovskite

The effect of the defect interface results is a critical impact on the performance of IPSC. In this work, the defect interface layers between GO/Perovskite have been considered. The defect interface layer types are neutral. For the first defect, total density which is integrated over all energies has been analyzed at the range of  $1 \times 10^7$  cm⁻² to  $1 \times 10^{18}$  cm⁻². A convergence failure in a simulation will happen if the defect interface value is too high.

# **3.5.3** The effect of capture cross-sections of electrons

The time between generation and recombination is the lifetime of carriers. In a studying of MAPbI₃ solar cells,  $\tau$  is the lifetime. It is found  $\tau$  the lifetime at range of 0.2-43.2 µs. The others report which is the perovskite absorber has been doped using bromine, MAPb ( $I_{0.71}Br_{0.29}$ )₃, the charge carrier lifetime increases (0.36-72.5 µs). In the other hands, the longer lifetime is depending on perovskite materials that have been doped with high-quality doping [34]. According to Equation (3.4),  $\tau_{n.p}$  is the electron (hole) lifetime, the lifetime depends on the capture cross-sections area for the density of the defect trap and for carrier.

$$\tau_{n.p} = \frac{1}{\sigma_{n,p} V_{th,n,p} N_t}$$
(3.4)

The capture cross-sections symbolized as the probability of the trap capturing the free carrier. The value of capture cross-sections of electrons varied from  $1 \times 10^{-19}$  cm² to  $1 \times 10^{-5}$  cm² which can affect the effect of the efficiency in IPSCs. In order

to obtain a better IPSC efficiency, analyzed the value of capture cross-sections of electron with doing simulation using SCAPS-1D software. If the value of capture cross-sections of electrons is too high, the efficiency of IPSC also reduced. The effect of capture cross-sections of holes

Effect of capture cross-sections of holes is same as capture cross-sections of electrons. It represents to the probability of the trap capturing the free carrier. The value of effect of capture cross-sections of holes also been considered. To begin with,  $1 \times 10^{-19}$  cm² to  $1 \times 10^{-15}$  cm² was examined to determine trends in IPSC efficiency. Even though it given a small change to the efficiency of IPSC, it has a strong bonding with capture cross-sections of electrons.

#### **3.5.4** The effect of working temperature

Temperature variables can be varied to influence the efficiency of IPSCs. To maximize IPSC efficiency, simulation can be used to change the working temperature. The temperature in this investigation was adjusted to a range of 300 K to 390 K. IPSC temperatures are measured in Kelvin. To test the performance of solar cells in a slightly cold environment, a minimum temperature of 300 K was chosen. Meanwhile, very hot conditions were tested at a maximum temperature of 390 K, whereas 300 K is the room temperature.

# 3.6 Taguchi Method

In this experiment, IPSC parameters should meet the performance specification such as  $V_{oc}$ ,  $J_{sc}$ , FF and PCE. One of the statistically methods for identifying the parameters, whose variability affect the effect of the IPSC performance is Taguchi method. Taguchi method has become a powerful tool for improving productivity during research and development. Taguchi method also can improve the quality of the

analyzed processes and products. The increment the number of process parameters, many experiments need to execute. The Taguchi method employs a unique design of orthogonal arrays to address this issue and explore the whole process parameter space with just a few experiments. The IPSC as GO as HTL optimization process flow is depicted in Figure 3.2.

# 3.6.1 Selection of Orthogonal Array

Orthogonal array (OA) can reduce the number of experimental. In order to choose an appropriate orthogonal array (OA) it depends on the total of parameter. In these experiments, L₉ OA was used. It has 9 experiments with 4 control factors. Taguchi L₉ OA greatly can reduce the number of tests and increase the efficiency. The experimental layout for the process parameters employing an orthogonal array of L₉  $(3^4)$  elements. The L₉ orthogonal array is used to comprehend the effect of four control factors whose levels were altered throughout nine rows of experiments.

UNIVERSITI TEKNIControl Factors YSIA MELAKA					
Expt. No.	A Thickness of GO	B Defect density of GO/Perovskite	C Capture cross- section of holes	D Capture cross- section of electrons	S/N Ratio (dB)
1	1	1	1	1	$\eta_1$
2	1	2	2	2	$\eta_2$
3	1	3	3	3	$\eta_3$
4	2	1	2	3	$\eta_4$
5	2	2	3	1	$\eta_5$
6	2	3	1	2	$\eta_6$
7	3	1	3	2	$\eta_7$
8	3	2	1	3	$\eta_8$
9	3	3	2	1	η ₉

Table 3.4: Experimental Layout Using L₉ (3⁴) Orthogonal Array

#### 3.6.2 Larger is Better

The target is to maximize the respond. The bigger the S/N, the better it is calculated to be. Since our aim is to maximize strength, the compressive strength in the current study should be higher. Equation (3.5) shows the  $\Pi$  for the quality characteristics of higher-the-better. The number of tests and experimental value of the obtained respond characteristics being represented as n and Yn respectively [29].

$$\Pi = -10 \log_{10} \left[ \frac{1}{n} \sum \left( \frac{1}{Y_{1^2}} + \frac{1}{Y_{2^2}} + \dots + \frac{1}{Y_{3^3}} \right) \right]$$
(3.5)

Experimentation can be utilized, for instance, to examine the influence of Factor A at level 3 (A₃). Level A3 of factor A was observed in experiments 7, 8, and 9. The average S/N ratio for these experiments, denoted by,  $m_{A_3}$  is calculated as follows [29]:

$$m_{A_3} = \frac{1}{3} \left[ \eta_7 + \eta_8 + \eta_9 \right]$$
(3.6)

Thus, the effect of Factor A at level  $A_3$  is given by  $(m_{A_3} - m)$  from Table 3.4; for experiments 7, 8, and 9, the level of Factor B is 1, 2, and 3, respectively. Similarly, the levels of Factors C and D had the values 1, 2, and 3 for these experiments. Therefore, the amount  $m_{A_3}$  reflects an average when the thickness of GO is at level  $A_3$ , where the averaging is performed in a balanced fashion across all levels of the other three components. The average S/N ratio for levels  $A_1$  and  $A_2$  of Factor A, as well as the ratios for the various levels of the other components, can be calculated in the same manner.

$$m_{B_2} = \frac{1}{3} \left[ \eta_2 + \eta_5 + \eta_8 \right]$$
(3.7)

The average S/N ratio at level  $B_2$  for Factor B. Due to the fact that the matrix experiment is built on an orthogonal array, all level averages share the same balancing property as  $m_{A_3}$ .

#### **3.6.3** Confirmation Experiment

In this experiment, initially 5 control factor was selected and  $L_8$  orthogonal array was used. It has 8 experiments with 5 control factors. However, the multiple result showed that only 4 control factors gave higher significant to S/N ratio compared to temperature always pooled or neutral in every process parameter. So  $L_9$  orthogonal array with 9 experiments and 4 control factors was selected.

The final step for the design of experiment process is the confirmation experiment. The aim of the confirmation experiment is to validate the analysis phase's conclusions [35]. Once the optimal level of process parameters has been determined, a confirmation test or final simulation is conducted to confirm the accuracy of the Taguchi Method prediction. The confirmatory test is unnecessary if the optimal combination of parameters and their levels coincides with one of the experiments in the orthogonal array. Using the following equations, the estimated value of the response characteristic under optimal conditions may be computed by adding the average performance to the contribution of each parameter at the optimal level [28]:

$$Y_{opt} = m + \sum_{i=1}^{n} (m_{iopt} - m)$$
(3.8)

Where m represents the average performance, n represents the number of process parameters or control variables, and  $m_{iopt}$  represents the average process parameter at the optimal level.

# **CHAPTER 4**

# **RESULTS AND DISCUSSION**

In this chapter will discuss regarding the outcome that has been successfully obtained from the simulation process in this project. Different parameter has been analyzed using Taguchi method  $L_9$  (OA) and the results will be discussed to obtain a better performance of the device. Then, all the parameters will be related with theory and discussed regarding problem faces during an experiment.

# 4.1 Analysis of layer thickness of GO

Analyzed the thickness of GO as HTL in order the improved the performance of IPSC. Initially, the thickness of GO has been varied from 10 nm to 100 nm. Table 4.1 shows a set of parameter value for four parameters which is PCE, FF,  $J_{sc}$  and  $V_{oc}$ . The trend of a varied thickness of GO layer for four parameters is illustrated in Figure 4.1. Based on Table 4.1, it can be observed that as the thickness of GO was varied from 10 nm to 100nm, the power conversion efficiency of IPSC decreases from 19.133% to 18.532%. As shown in Figure 4.1, the FF slightly raised from 81.360% to 81.481% due to the increase in GO thickness. The value of FF also depends on the value of  $J_{sc}$ 

and  $V_{oc}$ . The  $V_{oc}$  value is slightly increased from 0.935V to 0.942 V at 10 nm to 20 nm GO thickness and starts to decrease at 30 nm to 100 nm. Also, it was observed the value of  $J_{sc}$  is slightly decreased from 25.125 mA cm⁻² to 24.174 mA cm⁻².

GO thickness (nm) PCE (%) 10 18.181 20 19.133 30 19.065 40 18.980 50 18.899 60 18.821 70 18.745 80 18.672 90 18.601 100 18.532

Table 4.1: The Range of Thickness of GO



Figure 4.1: The Variation of GO Thickness on PCE, FF,  $J_{sc}$  and  $V_{oc}$ 

The thickness of GO cannot be too thin or too thick based on previous study. From previous research, HTL was applied to transport holes from the perovskite layer to the electrode by creating a barrier between the two substances. If HTL is excessively thick, the series resistance rises, and it becomes more difficult to transfer holes to the electrode. If HTL is too thin, it may not offer sufficient space between these layers. As a result, recombination will occur at the interface of the perovskite layer and electrode [14].

As an effect from Figure 4.1, the PCE are slightly decrease from 19.133% to 18.532% as the thickness increased from 20 nm to 10 nm. For an example, using GO as HTL on perovskite thin films in IPSC can improved the perovskite crystallization with enhanced hole extraction [35]. It concludes that, the variation in GO thickness can cause the efficiency slightly to increase.

#### 4.2 Analysis of an imperfection interface at GO/Perovskite layer

The interface between GO/Perovskite are very important in order to improve the performance of PCE. The higher the total density the lower the PCE. The defect density was varied from  $1 \times 10^7$  cm⁻² to  $1 \times 10^{18}$  cm⁻², cell parameters, the efficiency (PCE), voltage open circuit (V_{oc}), current short circuit (J_{sc}) and fill factor (FF) are significantly reduced [36].

The defect density parameters are illustrated in graph in Table 4.2. The influence of defect density of GO/Perovskite layer on the IPSC has been changed from  $1 \times 10^7$  cm⁻² to  $1 \times 10^{19}$  cm⁻² while the other variables were kept constant. It is seen in Figure 4.2, the increase in the defect density results in a slight decrease in the PCE, FF, J_{sc} and V_{oc}. It can also be noticed that the PCE decrease from maximum efficiency by about 77.270% and FF decreased from 81.729% by around 31.880% and  $J_{sc}$  decrement was less than 20.300% while  $V_{oc}$  decreased by around 58.130%.

Total Density (integrated over all	PCE (%)
energies) $(1/\text{ cm}^2)$	
$1 \times 10^{7}$	25.339
$1 \times 10^{8}$	22.910
$1 \times 10^{9}$	20.637
$1 \times 10^{10}$	18.532
$1 \times 10^{11}$	16.798
$1 \times 10^{12}$	15.238
$1 \times 10^{13}$	13.694
$1 \times 10^{14}$	11.984
$1 \times 10^{15}$	9.690
$1 \times 10^{16}$	7.055
$1 \times 10^{17}$	5.938
$1 \times 10^{18}$	5.776
1 × 10 ¹⁹	5.760
Sanno	

Table 4.2: The Range of an Imperfection Interface at GO/Perovskite Layer

The defect at the interfaces also can be called as recombination centers and it can affect the recombination process. If total density in interface GO/perovskites increased at the two interfaces, it will cause trapping and recombination which is it can reduce the performance of PSC. For PSC to obtain a good result, the defect density of GO/Perovskite must be less than or equal to  $1 \times 10^{12}$  cm⁻². The interface of GO/Perovskite influence the performance of IPSCs compared to interface between Perovskite/TiO2 [14]. The reaction between GO with perovskite surface can enhanced surface coverage and caused the films smoothness with fewer pinholes [37]. For an example, with using GO as an amphiphilic modifier, the photovoltaic performance of PSCs can be improved, and it can enhance the interface contact between perovskite

and the hole transport layer [38]. Solar cell performance decreases slightly due to the interface showing as defects when the defect density is varied over the test range.



Figure 4.2: The Variation of Defect Density of GO/Perovskite on PCE, FF, J_{sc} and V_{oc}

# 4.2.1 Analysis of capture cross-sections electrons.

Analyzed the value of capture cross-sections of electrons because it affects IPSC **UNVERSITITEKNIKAL MALAYSIA MELAKA** efficiency. Firstly, the value of capture cross-sections of electrons has been varied from  $1 \times 10^{-19}$  cm² to  $1 \times 10^{-5}$  cm². Table 4.3 shows a set of parameter value for four parameters which is PCE, FF, J_{sc} and V_{oc}. The graph of a varied value of capture cross-sections of electrons is illustrated in Figure 4.3.

The capture cross-sections represent the probability of the trap capturing the free carrier. As shown in Figure 4.3, if the value of capture cross-sections of electrons less than  $1 \times 10^{-9}$  cm² is almost constant whereas, if the value of capture cross-section increases from  $1 \times 10^{-19}$  cm² and above, the IPSC efficiency will decrease slightly from 18.532 % to 9.121 %. The value of FF greatly affects the increase in capture

cross-section area for electrons, where FF slightly decrease to  $1 \times 10^{-19}$  cm², however it was drastically reduced from 81.481 % to 50.162 % for higher capture cross-section area. The degradation of J_{sc} from 24.174 mA cm⁻² to 23.567 mA cm⁻² has been observe when capture cross-section was varied from  $1 \times 10^{-19}$  cm² to  $1 \times 10^{-5}$  cm². Additionally, it was noted that the V_{oc} decreased slightly from 0.941 V to 0.772 V when the capture cross-section area was raised.

Capture cross section electrons (cm ² )	PCE (%)
$1 \times 10^{-19}$	18.532
ALAYSIA 1×10 ⁻¹⁸	16.828
1 × 10 ⁻¹⁷	15.275
$1 \times 10^{-16}$	13.742
$1 \times 10^{-15}$	12.102
$1 \times 10^{-14}$	10.337
1 × 10 ⁻¹³	9.332
1×10 ⁻¹²	9.143
1×10 ⁻¹¹	9.122
$1 \times 10^{-10}$	9.121
UNIVERSITIE1×10-91 MALATS	9.121
$1 \times 10^{-8}$	9.121
$1 \times 10^{-7}$	9.121
$1 \times 10^{-6}$	9.121
$1 \times 10^{-5}$	9.121

Table 4.3: The Efficiency of IPSC at Different Value of Capture Cross-<br/>Sections of Electrons

For instance, the lower the capture cross-sections area for electrons, it will increase the carrier's lifetime and eventually increase the efficiency [38]. The lifetime of carriers is determined by the trap density and carriers capture cross-section. An increase in the cross-section, the carrier lifetime decreases. This is because dimension of defect trap increases leads to significantly decrease the solar cells performance [36]. Capture cross-section of electrons are not deflected and captured at defects in the ETL/Perovskite interface layer due to the moving electrons was move rapidly but in the HTL/Perovskite interface layer, the increased value of capture cross-section of electron will degrade the value of PCE. The coulombic force will slightly deflect the fastest carrier [39].



Figure 4.3: The Variation of Capture Cross-Sections of Electrons on PCE, UNIVERSITI TEKNIFF, J_{sc} and V_{oc}YSIA MELAKA

# 4.2.2 Analysis of capture cross-sections holes.

According to Table 4.4, the capture cross-section of holes values under  $1 \times 10^{-19}$  cm², the efficiency drops 18.532% to 18.509%. This is because the most significant processes in defect-assisted recombination losses. Defect with negatively charged will captured by holes due to the Coulomb interactions [39]. From Figure 4.4, increasing the value of capture cross-section influenced the FF where the value of FF increased slightly up to 81.481 % to 81.909 %. This is because the value of J_{sc} is almost constant at 24.174 mA cm⁻² compared to value of V_{oc} drops slightly from 0.941 V to 0.935 V.

Capture cross-	PCE (%)
sections holes (cm ² )	
$1 \times 10^{-19}$	18.532
$1 \times 10^{-18}$	18.511
$1 \times 10^{-17}$	18.509
$1 \times 10^{-16}$	18.509
$1 \times 10^{-15}$	18.509

Table 4.4: The Efficiency of IPSC at Different Value of Capture Cross-<br/>Sections of Holes



Figure 4.4: The Variation of Capture Cross-Sections of Holes on PCE, FF,  $J_{sc}$  and  $V_{oc}$ 

#### 4.2.3 Analysis of working temperature.

The temperature has been analyzed to see the performance of IPSC where it is related to thermal energy. Table 4.5 as shown the set parameter value for IPSC on the variation of working temperature. The graph obtained from the variation of working temperature of solar cell is also known in Figure 4.5 as shown.

Temperature (K)	PCE (%)
300	18.532
310	18.450
320	18.349
330	18.239
340	18.109
350	17.986
360	17.862
370	17.735
380	17.606
390	17.465

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 Table 4.5: The Efficiency of IPSC at Different Working Temperature

Based on Figure 4.5, it can be analyzed that as the working temperature increase, the efficiency of the solar cell will decrease from 18.532 % to 17.465 %. This is because up to 300 K and above freely moving electrons will move so rapidly. When free electrons move so rapidly, it will not pass through into PSC and current cannot flow. The benchmark between 300 K to 390 K can reduce the number of PCE, FF and  $V_{oc}$ . Meanwhile, the J_{sc} increase from 24.174 mA cm⁻² to 24.186 mA cm⁻² due to the increase in temperature.

For instance, the increase in temperature has an impact on  $J_{sc}$  to increase. In general, the reduction in PCE is from the increase of probabilities of recombination [40]. Due to the considerable energy absorption by the electrons at high temperatures, the performance of solar cells decreases as the temperature rises. A state of instability will then be reached by the electron. As a result, the rate of recombination before reaching the depletion region will rise and the efficiency of a solar cell would decrease.

Hence, the optimum working temperature of the device for IPSC with GO as HTL is 300 K where the efficiency of IPSC that has been achieved is 18.532 %.



Figure 4.5: The Variation of Working Temperature of PCE, FF, J_{sc} and V_{oc}

# 4.3 **Optimization using Taguchi Method AYSIA MELAKA**

The cell parameters were analyzed using Taguchi method  $L_9$  (3⁴) which has 9 experiments were used. The experimental layout for the four process parameters using  $L_9$  orthogonal array is shown in Table 4.6.

	Control Factors				
Fypt	А	В	С	D	S/N
No	Thickness	Defect density	Capture cross-	Capture	Ratio
110.	of GO	of	section of	cross-section	η (dB)
		GO/Perovskite	holes	of electrons	
1	1	1	1	1	$\eta_1$
2	1	2	2	2	$\eta_2$
3	1	3	3	3	$\eta_3$
4	2	1	2	3	$\eta_4$
5	2	2	3	1	$\eta_5$
6	2	3	1	2	$\eta_6$
7	3	1	3	2	$\eta_7$
8	WA'3AYSIA	2	1	3	$\eta_8$
9	3	3	2	1	η ₉
×		7			

Table 4.6: Experimental Layout using L₉ (3⁴) Orthogonal Array

In this section, the PCE, FF,  $J_{sc}$  and  $V_{oc}$  were analyzed. The process parameter settings were found using the Taguchi experimental design method. The control variables are important process parameters which is the thickness of GO, defect density of GO/Perovskite and the other two is capture cross-sections of holes and electrons. Three levels of treatment are applied to the four control factors. Because the effect of these parameters on the performance requirements may differ, three levels have been chosen.

Meanwhile, the two noise factors are thickness of Perovskites. Each of the noise factors was varied for 2 levels to obtain four reading of PCE, FF,  $J_{sc}$  and  $V_{oc}$  of experiment. The signal-to-noise ratio (S/N) is determined to study the elements that influence the response and interpret the measured study results. To enable a "bigger is better" response and provide high results, the best value for each selected experience

was determined by comparing the signal-to-noise ratio (S/N) [41]. Therefore, the process parameter fluctuation can be improved by selecting the right testing condition (noise factor settings) during Robust Design experiments. Tables 4.7 and 4.8, respectively, list the values of the process parameter and noise factor at various levels.

 Table 4.7: Process Parameters and The Levels

		LEVELS	
LEVELS	1	2	3
Thickness of GO (A)	80	90	100
Defect density of GO/Perovskite (B)	1 × 10 ⁸	1 × 10 ⁹	$1 \times 10^{10}$
CCS Holes (C)	$1 \times 10^{-19}$	$1 \times 10^{-18}$	$1 \times 10^{-17}$
CCS Electrons (D)	$1 \times 10^{-19}$	$1 \times 10^{-18}$	$1 \times 10^{-17}$

#### **Table 4.8: Noise Factors and The Levels**

NOISE FACTORS \ LEVELS	Noise Level 1	Noise Level 2	Number of Levels
Thickness of Perovskite 1	1000	و مر 1100 ي	2
Thickness of Perovskite 2	NIKA1200 AL	VISI1300 ELA	<b>KA</b> 2

Nine different experiments using the design parameter combinations in the provided orthogonal array table, on the thickness of GO, defect density of GO/Perovskite, capture cross-section holes, and capture cross-section electrons were performed. For each set of parameter combinations, four experiments were simulated. The next stage is to identify which control parameters can have an impact on a device characteristic after the response for PCE data using the L₉ array has been completed. The most effective combinations were quickly identified using the signal-to-noise (S/N) ratio. PCE of IPSC devices is one of the larger-the-best quality parameters in

this study. This signal-to-noise (S/N) ratio was used as reference in order to determine the value of PCE after using L₉ array predict or not.

# 4.3.1 **Optimization of PCE in IPSC devices**

Table 4.9 illustrates the PCE findings for the IPSC device employing the  $L_9$  orthogonal array. The next stage is to establish the required values for a few parameters, including the thickness of GO, the defect density of GO/Perovskite, the capture cross-section of electrons, and the capture cross-section of holes that had an impact on a device.

	Repetiti	ions or Measu	rements for ea	ch expt						
Expt.										
No.	1 8	2	3	4						
E 1	23.191	23.357	23.488	23.592						
2	19.238	19.365	19.463	19.540						
3	16.921	17.013	17.080	17.126						
يا ملاك	20.714	20.858	20.971	21.060						
	20.615	20.758	20.869	20.957						
6	17.382	17.484	17.560	17.615						
7	21.216	21.365	21.482	21.575						
8	18.796	18.922	19.019	19.094						
9	18.511	18.631	18.722	18.793						

 Table 4.9: PCE Values for IPSC Devices

Based on Table 4.10, it shows the value of S/N ratio the quality characteristics is larger-the-better. By using Eqn. 3.6, the η for each experiment was calculated.

Mean Sum of Squares of reciprocals	S/N Ratio			
	(Larger-the-Better)			
$1.83 \times 10^{-3}$	27.39			
$2.66 \times 10^{-3}$	25.76			
$3.45 \times 10^{-3}$	24.63			
$2.29 \times 10^{-3}$	26.40			
$2.31 \times 10^{-3}$	26.36			
$3.26 \times 10^{-3}$	24.87			
$2.18 \times 10^{-3}$	26.61			
$2.78 \times 10^{-3}$	25.56			
$2.87 \times 10^{-3}$	25.42			

 Table 4.10: S/N respond for the PCE

Orthogonal is used as the experimental design, the effect of each process parameter on the S/N Ratio at various levels may be distinguished. Table 4.11 summarizes the S/N ratio for each level of the process parameters. In addition, the overall mean S/N ratio for the nine studies is computed and presented in Table 4.11.

CONTROL FACTORS \LEVELS	CONTROLLEVELSDegreesFACTORS0fLEVELS123Freedom		Sum of Squares	Mean Square	Factor Effect (%)	Empty or pooled		
Thickness of								F=<1.3
GO (A)	25.92	25.88	25.86	2	0	0	0	Pooled
Defect density of GO/ Perovskite (B)	26.80	25.89	24.97	2	5	3	80	No
Capture cross- section holes (C)	25.94	25.86	25.87	2	0	0	0	Pooled
Capture cross- section electrons (D)	26.39	25.74	25.53	2	1	1	19	No

Table 4.11: The Values Obtained of ANOVA for PCE in IPSC Devices

In Table 4.11 shows the result of ANOVA for PCE in IPSC devices. Generally, the PCE quality characteristic improves as the S/N ratio increases. The closer the quality characteristic value is to the target, the higher the quality of the product [28]. For PCE, control factors thickness of GO (Factor A), defect density of GO/Perovskite (Factor B), capture cross-section holes (Factor C) and capture cross-section electrons (Factor D) were found level 1 as dominant factor because it has maximum S/N Ratio (η). In addition, the control factor B has more effect on PCE IPSC because the factor effect is 80% and the control factor D is only 19%. Whereas the control factors A and C are 0% which means it does not affect the PCE of the IPSC device. Figure 4.6 show the S/N Ratio (Larger-the-best) graphs where he dashed line is the value of the total mean of the S/N ratio and the other is factor effects. This graph is illustrated from Table 4.11 which is that the higher the level of the control factor is the dominant factor because it has the maximum S/N Ratio (η).



Figure 4.6: S/N Graph of PCE for IPSC Devices

Table 4.12 as shown that the level that have been selected due to the higher S/N ratio. The final step, following the selection of the ideal level of process parameters, is to predict and validate the improvement of the performance characteristic using the optimal level of process parameters. The S/N ratio of optimum level of the process parameters is 27.39 which is predict to the performance characteristics.

CONTROL		LEVELS				Factor	Dominant/
FACTORS	1	2	2	level	Name	Effect	Significant/Neutral
\LEVELS	1	2	3			(%)	C
Thickness of	80	90	100	1	_	0	Neutral
GO (A)	00	90	100	1	-	U	Neutrai
Defect density	WALAYS	14					
of	$1 \times 10^{8}$	$1 \times 10^{9}$	$1 \times 10^{10}$	1	$1 \times 10^8$	80	Dominant
GO/Perovskite	17. 20		1 / 10		14 10	00	Dominum
(B)		2					
Capture cross-		× 10	15	1		V.I	
section holes	$1 \times 10^{-19}$	$1 \times 10^{-18}$	$1 \times 10^{-17}$	1	I V	0	Neutral
(C)							
Capture cross-							
section	$1 \times 10^{-19}$	$5 \times 10^{-19}$	$10 \times 10^{-19}$	1	1 x 10 ⁻¹⁹	19	Dominant
electrons (D)							
S/N Rat	lo lu	ulo Le	1	27	.3	sau a	
5/11/144	10	- 27	.44		5. 0	1.1	27.16

Table 4.12: Predict S/N Ratio of PCE in IPSC Devices

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# 4.3.2 **Optimization of FF in IPSC devices**

The results of FF in IPSC device using  $L_9$  orthogonal array is shown in Table 4.13. After nine experiments of  $L_9$  array have been performed, the value of S/N ratio have been calculated by using Eqn. 3.6 as shown in Table 4.14.

Expt.	Repetitions or Measurements for each expt.									
No.	1	2	3	4						
1	81.310	81.301	81.290	81.279						
2	81.371	81.312	81.254	81.197						
3	82.676	82.524	82.371	82.216						
4	80.984	80.952	80.921	80.890						
5	81.250	81.217	81.183	81.150						
6	81.246	81.124	81.003	80.881						
7	81.202	81.176	81.151	81.125						
8	79.314	79.258	79.202	79.146						
9 ALAI	81.864	81.789	81.715	81.641						

**Table 4.13: FF Values for IPSC Devices** 

Based on Table 4.14, it shows the S/N ratio value for the quality characteristics is larger-the-better.

ويبو Table 4.14: S/N Respond for the FF

U	Mean Sum of Squares of reciprocals	S/N Ratio (Larger-the-Better)
	$1.51 \times 10^{-4}$	38.20
	$1.51 \times 10^{-4}$	38.20
	$1.47 \times 10^{-4}$	38.32
	$1.53 \times 10^{-4}$	38.16
	$1.52 \times 10^{-4}$	38.19
	$1.52 \times 10^{-4}$	38.18
	$1.52 \times 10^{-4}$	38.19
	$1.59 \times 10^{-4}$	37.98
	$1.50 \times 10^{-4}$	38.25

Table 4.15 summarizes the S/N ratio for each level of the process parameters. Then, the overall mean S/N ratio for the nine studies is determined and displayed in Table 4.15.

CONTROL FACTORS \LEVELS	1	LEVELS	3	Degrees of Freedom	Sum of Squares	Mean Square	Factor Effect (%)	Empty or pooled F=<1.5
Thickness of GO (A)	38.24	38.18	38.14	2	0	0	24	No
Defect density of GO/ Perovskite (B)	38.18	38.12	38.25	2	0	0	36	No
Capture cross- section holes (C)	38.12	38.20	38.23	2	0	0	32	No
Capture cross- section electrons (D)	38.21	38.19	38.15	2	0	0	8	No

Table 4.15: The Values Obtained of ANOVA for FF in IPSC Devices

For FF in IPSC devices, the defect density of GO/Perovskite (Factor B – 36%) and the capture cross-section of holes (Factor C – 32%) were determined to be the main factor influencing fill factor, FF. This is because Factors B and C have high percent effect compared to other control factors. The percent effects on S/N ratio of thickness of GO and capture cross-section of electrons are much lower being 24% and 8% respectively. The analysis of average performance indicates the optimum condition to be  $A_1B_3C_3D_1$ .

Figure 4.7 shows the S/N Ratio (Larger-the-best) graphs where each control factors with the higher S/N Ratio ( $\eta$ ) is the dominant factor. The dashed line the value of the total mean of the S/N ratio and the straight line is factor effects.





The level that was chosen because of the increased S/N ratio is shown in Table 4.16. The final stage is to predict and confirm the increase in the performance characteristic using the optimal level of the process parameters once the optimal level of the process parameters has been chosen. The optimal S/N ratio for the process parameters is 38.25 which is approximately to the predict value 38.30.

CONTROL		LEVELS		Qui	τ1	Factor	Devicest	
FACTORS \LEVELS	1	2 3		level	Level Name	Effect (%)	Significant/Neutral	
Thickness of GO (A)	80	90	100	1	80	24	Dominant	
Defect density of GO/Perovskite (B)	1×10 ⁸	1 × 10 ⁹	$1 \times 10^{10}$	3	1x 10 ¹⁰	36	Dominant	
Capture cross- section holes (C)	1×10 ⁻¹⁹	$1 \times 10^{-18}$	1× 10 ⁻¹⁷	3	1 x 10 ⁻¹⁷	32	Dominant	
Capture cross- section electrons (D)	1× 10 ⁻¹⁹	5× 10 ⁻¹⁹	$10 \times 10^{-19}$	1	1 x 10 ⁻¹⁹	8	Significant	
S/N Ratio				38	.4			
5,1 ( <b>Ru</b> tio		38	3.46				38.30	

Table 4.16: Predict S/N Ratio of FF in IPSC Devices

# 4.3.3 Optimization of J_{sc} in IPSC Devices

Table 4.17 displays the results of the  $J_{sc}$  in the IPSC device utilizing the  $L_9$  orthogonal array. After nine experiments from  $L_9$  array have been completed, the next stage is to identify the required values for chosen parameters, including the thickness of GO, defect density of GO/Perovskite, capture cross-section of electrons and capture cross-section of holes, which had an effect on the device.

E. M.	Repetitions or Measurements for each expt.								
Expt. No.	1	2	3	4					
1 MALA	24.350	24.519	24.654	24.762					
2 2	24.350	24.519	24.654	24.762					
<b>EK</b>	24.350	24.519	24.654	24.762					
E 4	24.261	24.430	24.565	24.673					
5 100	24.261	24.430	24.565	24.673					
6	24.261	24.430	24.565	24.673					
با ملاك	24.174	24.344	24.478	24.587					
	24.174	24.344	24.478	24.587					
9	24.174	24.344	24.478	24.587					

 Table 4.17: The Values of J_{sc} for IPSC Devices

According to Table 4.18, the higher the S/N ratio, the higher the quality characteristics. By using Eqn. 3.6, the  $\eta$  for each experiment was calculated. The orthogonal experimental design allows for the separation of the effects of each process parameter on the S/N Ratio at various levels.

Mean Sum of Squares of reciprocals	S/N Ratio (Larger-the- Better)
$1.66 \times 10^{-3}$	27.81
$1.66 \times 10^{-3}$	27.81
$1.66 \times 10^{-3}$	27.81
$1.67 \times 10^{-3}$	27.78
$1.67 \times 10^{-3}$	27.78
$1.67 \times 10^{-3}$	27.78
$1.68 \times 10^{-3}$	27.75
$1.68 \times 10^{-3}$	27.75
$1.68 \times 10^{-3}$	27.75

Table 4.18: S/N Respond for the J_{sc} of Nine Experiments

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Table 4.19 provides an overview of the S/N ratio for each level of the process parameters. Additionally, table 4.19 provides the total mean S/N ratio for the nine tests once the value has been determined.

CONTROL	RSITLEVELS			Degrees	SiA MI	ELAKA Mean	Factor	Empty or
FACTORS     \LEVELS	1	2	3	of Freedom	Squares	Square	Effect (%)	pooled F=<1.5
Thickness of GO (A)	27.81	27.78	27.75	2	0	0	24	No
Defect density of GO/ Perovskite (B)	27.78	27.78	27.78	2	0	0	36	No
Capture cross- section holes (C)	27.78	27.78	27.78	2	0	0	32	No
Capture cross- section electrons (D)	27.78	27.78	27.78	2	0	0	8	No

Table 4.19: The Values Obtained of ANOVA for J_{sc} in IPSC Devices

For  $J_{sc}$  in IPSC devices, the most effective process parameters with respect to the performance of IPSC devices are thickness of GO (Factor A – 100%). According to the Table 4.19, thickness of GO was found to be the major factor affecting the performance of IPSC compared to other control factors (0%). An effect control factors 0% that it does not affect the short-circuit current,  $J_{sc}$ . The analysis of average performance indicated that the optimal condition existed is  $A_1B_1C_1D_1$ .



The S/N Ratio (Larger-the-Best) graphs are shown in Figure 4.8, with the factor effects represented by the straight line and the total mean of the S/N ratio represented by the dotted line. As depicted by this graph, which is taken from Table 4.19, the greater the level of the control factor, which has the highest S/N Ratio ( $\eta$ ), the more dominant factor it is. For instance, thickness of GO (Factor A) has the highest S/N Ratio ( $\eta$ ), compared to others control factors at same level of the total mean.

CONTROL FACTORS \LEVELS		LEVELS			X 1	Factor	Dominant/ Significant/Neutral	
	1	2	3	level	Level Name	Effect (%)		
Thickness of GO (A)	80	90	100	1	80	100	Significant	
Defect density of GO/Perovskite (B)	1× 10 ⁸	$1 \times 10^{9}$	$1 \times 10^{10}$	1	-	0	Neutral	
Capture cross- section holes (C)	1×10 ⁻¹⁹	$1 \times 10^{-18}$	1×10 ⁻¹⁷	1	-	0	Neutral	
Capture cross- section electrons (D)	1× 10 ⁻¹⁹	5× 10 ⁻¹⁹	$10 \times 10^{-19}$	1	-	0	Neutral	
S/N Ratio				27	.8			
S/1 Y Rutto		27	.86			27.76		

Table 4.20: Predict S/N Ratio of J_{sc} in IPSC Devices

For  $J_{sc}$  in IPSC devices, thickness of GO (Factor A -100%) were defined as the major factor affecting the  $J_{sc}$  in IPSC. The factor A effect was 100% compared to other factor effect which is 0% or neutral was found not significant to the short-circuit current,  $J_{sc}$ . The optimal S/N ratio for the process parameter, which predicts the performance characteristics, is 27.8.

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# 4.3.4 Optimization of Voc in IPSC Devices

The results of  $V_{oc}$  in IPSC device using L₉ orthogonal array is depicted in Table 4.21. After nine experiments of L₉ array have been implemented, the value of S/N ratio have been calculated by using Equation (3.6) as shown in Table 4.22.

Evet No	Repetitions or Measurements for each expt.						
Expl. No.	1	2	3	4			
1	1.171	1.172	1.172	1.172			
2	0.971	0.971	0.972	0.972			
3	0.841	0.841	0.841	0.841			
4	1.054	1.0547	1.055	1.055			
5	1.046	1.0462	1.046	1.047			
6	0.881	0.882	0.882	0.883			
7	1.081	1.081	1.081	1.082			
8	0.980	0.981	0.981	0.981			
9 ALAYS	0.935	0.936	0.936	0.936			

Table 4.21: V_{oc} Values for IPSC Devices

Based on Table 4.26, it shows the value of S/N ratio the quality characteristics is larger-the-better. By using Eqn. 3.6, the  $\eta$  for each experiment was calculated.

JNIV	Mean Sum of Squares of reciprocals	S/N Ratio (Larger-the- Better)
	$7.28 \times 10^{-1}$	1.38
	1.06	-0.25
	1.41	-1.51
	$8.99 \times 10^{-1}$	0.46
	$9.13 \times 10^{-1}$	0.39
	1.28	-1.09
	$8.55 \times 10^{-1}$	0.68
	1.04	-0.17
	1.14	-0.58

# Table 4.22: S/N Respond for the V_{oc} for Nine Experiments

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In this experiment as mentioned, with using  $L_9$  orthogonal array, it is possible to isolate the effect of each process parameter on the S/N ratio at various levels. As depicted in Table 4.23, the S/N ratio for each level of the process parameter is summarized.

CONTROL FACTORS \LEVELS	1	LEVELS	3	Degrees of Freedom	Sum of Squares	Mean Square	Factor Effect (%)	Empty or pooled F=<1.5
Thickness of GO (A)	-0.13	-0.08	-0.02	2	0	0	0	Pooled
Defect density of GO/ Perovskite (B)	0.84	-0.01	-1.06	2	5	3	83	No
Capture cross- section holes (C)	0.04	-0.12	-0.14	2	0	0	1	Pooled
Capture cross- section electrons (D)	0.40	-0.22	-0.40	2	T	1	16	No

Table 4.23: The Values Obtained of ANOVA for Voc in IPSC Devices

For open-circuit voltage,  $V_{oc}$  in IPSC devices, defect density of GO/Perovskite (Factor B + 83%) and capture cross-section of electrons (Factor D - 16%) were deemed to be the main influence on the  $V_{oc}$ . This is because Factors B and D have high percent contribution compared to other factors. The percent effects on S/N ratio of thickness of GO and capture cross-section of holes are much lower being 0% and 1% respectively. According to Table 4.23, defect density of GO/Perovskite found to be major factor affecting the  $V_{oc}$  in IPSC devices. The analysis of average performance indicated that the optimum condition is  $A_3B_1C_1D_1$ . Figure 4.9 show the S/N Ratio (Larger-the-best) graphs in which the dashed line represents the total mean of the S/N ratio, and the other line is factor effects. The higher the level of the control factor is the dominant factor due to the maximum of S/N Ratio ( $\eta$ ).



As depicted in Table 4.24 shows the level have been selected due to the higher S/N ratio. Once the optimal level of the process parameters has been chosen and proceed to the final step which is predict and verify the S/N ratio optimum level of the process parameters. The value of S/N ratio optimum level of the process parameters is 1.37 which is predict to the performance characteristics.

CONTROL		LEVELS		Qui	<b>X</b> 1	Factor	Dominant/
FACTORS \LEVELS	1	2	3	level Name		Effect (%)	Significant/ Neutral
Thickness of GO (A)	80	90	100	3	-	0	Neutral
Defect density of GO/Perovskite (B)	1× 10 ⁸	1 × 10 ⁹	$1 \times 10^{10}$	1	1x 10 ¹⁰	83	Dominant
Capture cross- section holes (C)	1×10 ⁻¹⁹	$1 \times 10^{-18}$	1×10 ⁻¹⁷	1	-	0	Neutral
Capture cross- section electrons (D)	1× 10 ⁻¹⁹	5×10 ⁻¹⁹	$10 \times 10^{-19}$	1	1 x 10 ⁻¹⁹	16	Dominant
S/N Ratio				1.3			
		1.59				1.03	

Table 4.24: Predict S/N Ratio of Voc in IPSC Devices

# 4.4 Multiple Optimization

Based on individual results from PCE, FF,  $J_{sc}$  and  $V_{oc}$ , the average performance analysis from each parameter was recorded. Each parameter shows the optimum level was chosen because of the higher S/N ratio. The percent effect on the S/N ratio indicates the dominant factor to the process parameter. From Table 4.25, it shows the multiple optimization results.

Parameters	А	В	С	D	Average
PCE (%)	1 (0%)	1 (80%)	1 (0%)	1 (19%)	23.407
FF (%)	1 (24%)	3 (36%)	3 (32%)	1 (8%)	81.781
J _{sc} (mA/cm2)	1 (100%)	1 (0%)	1 (0%)	1 (0%)	24.571
V _{oc} (V)	3 (0%)	1 (8%)	1 (1%)	1 (16%)	1.171
Multiple Optimization	1	1	1	1	

 Table 4.25: The Level Obtained for Multiple Optimization in IPSC Devices

Based on Table 4.25, the four control factors on each parameter namely PCE, FF,  $J_{sc}$  and  $V_{oc}$  show the percent effect on the S/N ratio. Firstly, the thickness of GO (Factor A) is selected level 1 (80nm) when it has more effect on  $J_{sc}$  due to the higher percent effect is 100% compared to level 3 only 0% effect to  $V_{oc}$ . Next, the defect density of GO/Perovskites (Factor B), level 1 is the higher percent effect which is 80% compared to level 3 only 36%. So, for defect density of GO/Perovskites level 1 (1 x 10⁸ cm⁻²) was chosen. Further, for capture cross-section of holes (Factor C), level 1 was chosen even though the percentage of effect is 0% compared to level 3 which is 32%. This is because, in this experiment, first priority if more focused on PCE in IPSC compared to other parameters. Lastly, level 1 is selected for capture cross-section of electrons (Factor D) because all parameters was chosen level 1 as the dominant factor.

Parameters	Initial IPSCs	Optimized IPSCs
Thickness of GO (nm)	100 5.	80
Defect Density of KNI GO/Perovskite	KAL 1×10 ¹⁰ SIA	/ELA1×10 ⁸
Capture cross section electrons (cm ² )	$1 \times 10^{-19}$	$1 \times 10^{-19}$
Capture cross section holes (cm ² )	$1 \times 10^{-19}$	$1 \times 10^{-19}$

**Table 4.26: Parameter Before and After Optimization** 

From Table 4.26 above, it shows each parameter that has been used before and after optimization. The GO thickness value after optimization is 80 nm thinner than before optimization due to the thicker HTL, the series resistance, Rs increases and the transfer of holes to the electrode becomes more difficult. Next, to obtain a higher PCE in IPSC devices above 25%, the GO/Perovskite defect density value should be
considered. The cross-sectional capture of electrons and holes does not require any changes as  $1 \times 10^{-19}$  cm² is commonly used from other research.

Parameters	Before Optimization	After Optimization		Previous
		Individual	Multiple	Journal [1]
PCE (%)	18.530	23.407	23.407	16.51
FF (%)	81.480	81.782	81.295	81.490
J _{sc} (mA/cm2)	24.174	24.572	24.571	21.710
V _{oc} (V)	0.941	1.171	1.172	0.930

Table 4.27: Comparison of Values Obtained Before and After Optimization



Figure 4.10: Comparison of Values Obtained Before and After Optimization

Based on Figure 4.10, the comparison results before and after optimization show the value of PCE increase in IPSC devices. Before optimization PCE is 18.530% compared to after optimization PCE value is 23.407%.



Figure 4.11: Comparison Values Obtained Before and After Optimization for of PCE, FF, J_{sc} and V_{oc} of IPSC

As illustrated from Table 4.27 and Figure 4.11, the results obtained after optimization were improved compared to before optimization. The PCE has achieved the optimum efficiency which is at 23.407 %. Furthermore, the  $J_{sc}$  and  $V_{oc}$  were improved after optimization to 24.571 mA/cm2 and 1.172 V respectively. This is because modification of process parameters can increase quality, and the optimal process parameters found using the Taguchi method are insensitive to ambient variables and other noise factors [42]. Fill factor, FF were slightly decrease from 81.480 % to 81.295 % due to the certain control factors have been selected according to the PCE. After optimization result is divided by two which is one for individual parameter result and the other one for multiple result or final result.

#### 4.5 Environment and sustainability

In terms of the environment, a solar cell is well-known as the cleanest energy source. In contrast to fossil-fuel-generated electricity, a solar cell is very effective at maximizing the production of electricity and minimizing carbon emissions. Next, in the aspect of sustainability, the electricity produced by the solar cell is more sustainable compared to fossil fuel since sunlight is always readily available at no cost. In addition, this project does not consume any cost since it is entirely simulated using SCAPS-1D software and optimize using Taguchi method.



# **CHAPTER 5**

## **CONCLUSION AND FUTURE WORKS**

This chapter will discuss the overall conclusion by providing the overall summary of the project. Future works also will be suggested.

### 5.1.1 Conclusion

IPSC is a type of perovskite solar cells having n-i-p (regular) and p-i-n (inverted). The placement of HTL and ETL is what differentiates these two topologies. For the perovskite solar cells with inverted structure (IPSC) the HTL layer place on top of TCO (transparent conducting oxide) substrate. By employing GO as HTL in IPSC, the performance of IPSC is encouraging as GO offers high charge mobility, reliability, low processing cost, large-scale production possibilities, and good dispersibility in a variety of solvents.

The main objective of this project which is to simulate GO as HTL on a solar cell using SCAPS-1D simulation software was succeeded. The simulation was implemented by employing a complete simulated device structure composed of FTO/GO/  $CH_3NH_3PbI_3$ /  $TiO_2/Ag$ . Besides, the analysis of this project which is to optimize GO as HTL also was successfully performed. Several key parameters of HTL have been analyzed to obtain the optimum performance for IPSC as well as the influence of back contact.

The simulation results showed that GO as HTL in IPSC has produced an efficiency 18.53% compared to previous researcher of methylammonium lead triiodide perovskite solar cell (PSC) containing graphene oxide (GO) as HTL has achieved an optimal PCE of 16.51% using SCAPS-1D simulation. In additionally, after optimization using Taguchi Method L₉ OA the efficiency increased to 23.408 %. This is shows that the optimum solution in achieving the desired efficiency in IPSC devices was successfully predicted by using Taguchi Method. Overall, the project was a success. The efficiency can be improved by using GO as HTL in IPSC devices and optimizing it using Taguchi Method.

# 5.1.2 Future works

In The future, the optimization results can be used as a guide in the fabrication process for IPSC employing GO as hole transport layer. The performance of GO as HTL in IPSC device can be improved by do analysis on defect density of ETL/Perovskite layer.

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