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SCAPS NUMERICAL ANALYSIS OF GRAPHENE OXIDE/TIO$_2$ BULK HETEROJUNCTION SOLAR CELL SENSITIZED BYN719 RUTHENIUM DYE[†]

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Solid-state dye-sensitized solar cells (SSDSC) have been fabricated using two different metal oxide materials, graphene oxide and titanium oxide, are used as hole and electron transport materials, respectively. The N719 dye ruthenium between the hole and electron transport materials to act as an absorber layer in your Go/N719dye/TiO$_2$ solar cells. Through the SCAPS-1D simulation, it was found that the Go/N719dye/TiO$_2$ solar cells have significantly improved the performance of the solar cells compared to the Go/TiO$_2$ solar cells. Specifically, the short circuit current (Jsc) has increased from 0.17 mA/cm^2 to 1 mA/cm^2, the open circuit voltage (Voc) has increased from 0.2 V to 1 V, and the power conversion efficiency (η) has increased from 0.02% to 2.5%. Additionally, Various factors that can affect the performance of Go/N719 dye/TiO$_2$ solar cells. It was found that the optimal dye thickness for achieving high short circuit current density, high power conversion efficiency, and high open circuit voltage is between 200nm and 300nm. Furthermore, the operating temperature of the solar cells also affects their performance. Increasing the operating temperature negatively affects the open circuit voltage and power conversion efficiency of the cells, while the short circuit current density is slightly enhanced. Finally, the efficiency of a solar cell can be affected by the type of metal used for the electrode and the type of semiconductor material used in the cell. In Ni and Cu electrodes solar cells ohmic contacts allow for efficient transfer of electrons, whereas Schottky barriers can impede electron flow and reduce efficiency in Mo and Ag electrodes solar cells.

Keywords: *SCAPS; Graphene oxide; Operating temperature; Thickness; Work function; Parameter of solar cells*
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1. INTRODUCTION

Photovoltaic (PV) technology is used to convert sunlight into electricity, and it typically involves the use of solar cells made of semiconductor materials such as silicon [1.2] Hybrid photovoltaic cells have different semiconductor layers and junctions that allow them to create hole-electron pairs more efficiently, which leads to better performance such as Dye-sensitized solar cells (DSSCs). This device is a specific type of hybrid PV cell that uses a layer of organic dye to absorb light and create electron-hole pairs, which are then transported to an electrode by a layer of inorganic Nano-crystalline material [2-4]. They several advantages over traditional silicon-based solar cells, including lower production costs and the ability to generate electricity in low-light conditions. However, they also have some limitations, such as lower efficiency and shorter lifespan. Nevertheless, DSSCs are a promising technology that could help to make solar energy more accessible and affordable in the future [4].

The common hole conductor used in fabricating dye-sensitized MOSCs (Metal-Oxide-Semiconductor Cells) is an electrolyte composed of an iodine couple dissolved in an organic solvent [3,5]. This electrolyte plays a crucial role in the functioning of the MOSCs by providing the pathway for the transport of holes from the dye to the electrode. However, as known, there are certain problems associated with using electrolyte as the hole conductor. One of the main issues is the requirement for a good seal to prevent any leakage of the electrolyte, which can be challenging to achieve over long periods of time [5]. This leakage can not only affect the performance of the MOSCs but can also pose safety risks. To overcome this problem, researchers have been exploring alternative hole conductors, such as solid-state hole conductors or organic hole-transporting materials. These materials can offer improved stability and reliability compared to electrolytes, while also reducing the risk of leakage and increasing the lifetime of MOSCs. For example, solid-state materials such as PEDOT: PSS have been investigated as an alternative to electrolytes as the hole conductor in MOSCs. PEDOT:PSS has several advantages, such as high work function, high conductivity, high optical transmittance, easy solution process ability, and potential application on flexible substrates, which make it an attractive material for MOSCs and other solar cell application [6]. Recently m Yuhan Wu produced high efficiency solar cells of 18% utilizing bromide (KBr) into poly (3,4-ethylenedioxythiophene): polystyrene sulfonate) (PEDOT:PSS) to improve its own conductivity and interfacial charge transfer [7]. On other hand, there are also some drawbacks to using PEDOT:PSS as a hole transport layer. PEDOT:PSS can also be sensitive to moisture, leading to decreased performance and stability over time [8]. As a result, researchers are actively exploring alternative hole transport materials that can offer better performance, stability, and cost-effectiveness. Some promising options include metal oxides (such as TiO$_2$ or SnO$_2$), conjugated polymers (such as PTB7 or P3HT), and carbon-based materials (such as graphene or carbon nanotubes). Graphene oxide (GO) has been investigated as a potential alternative to PEDOT:PSS as a hole transport material in solar cells. GO has several interesting properties, including a band gap energy of 3.5 eV, excellent transparency, low production cost, large scale production

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capability, good solubility in many solvents, and high hole mobility [5,8]. Due to these properties, GO has been demonstrated to be a promising material for improving the efficiency of solar cells. Its high transparency allows for more light to pass through the cell and be absorbed by the active layer, while its high hole mobility can facilitate the transport of charge carriers and reduce the recombination of electrons and holes. Other important part in DSSCs is ruthenium dyes. It has indeed been extensively studied in photochemistry due to their remarkable properties such as chemical stability, excited state reactivity, luminescence, and long excited state lifetime [9,10].

This study aims to examine various factors that affect the performance of the solar cell, such as the presence of N719 Ruthenium dye, the thickness of the dye layer, the work function of the back contact, and the temperature. This information can provide insights into optimizing the design and performance of the solar cell. SCAPS-1D simulation package is a powerful tool for modeling the physical and electrical behavior of solar cells, including the absorption of light, generation and transport of charge carriers, and recombination processes [11]. It can simulate the effect of different parameters on the device performance, allowing for the optimization of the solar cell design.

2. NUMERICAL MODELING AND STRUCTURE DEVICE

Solar Cell Capacitance Simulator (SCAPS-1D) is a one-dimensional solar cell simulation program developed by the department of Electronics and Information Systems (ELIS) at the University of Gent, Belgium [11]. The purpose of SCAPS-1D is to simulate and evaluate the performance of Single-Step Deposition-Synthesized Solar Cells (SSDSC). It is also capable of modeling a variety of solar cell parameters and characteristics, including electrical and optical properties, interface and bulk recombination, and temperature and illumination dependence. SCAPS-1D uses a drift-diffusion approach to simulate carrier transport and considers the effects of doping, carrier lifetime, and surface recombination velocity on the cell's performance. The program has been validated against experimental data and has been used in various research studies to analyze the performance of different types of solar cells. Initially, the program was used to simulate the performance of solar cells made of $CuInSe_2$ and CdTe materials [11]. Later on, researchers began using the program to simulate the performance of crystalline solar cells and other types of materials [12].

This work has utilized SCAPS, a modeling software for solar cells, to investigate how certain parameters of the cells are affected by varying factors. Specifically, the thickness of the dye layer, operating temperature, and work function of the back contact were examined, and the efficiency, short circuit current density, and fill factor were extracted as parameters of interest. This was accomplished by analyzing the current density versus voltage of the solar cells under different experimental conditions. The SSDSC is a layered structure consisting of main layers): Graphen oxide (Go), nano crystalline Titanium oxide (TiO_2), N719 Ruthenium Dye, back contact and front contact. Figure 1 show schematic diagrams of TiO_2/dye/Go solar cells.

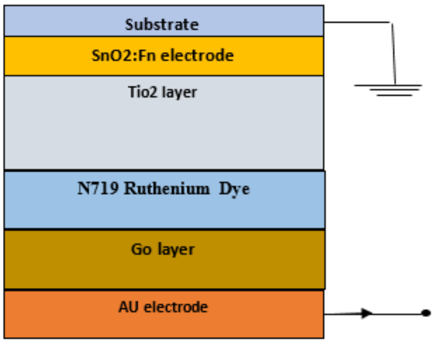


Figure 1. Schematic of the GO/N719dye/nc-TiO_2 solar cells

From previous literatures (13-15) Tables 1 and 2 present the input parameters used in SCAPS simulators for studying the performance of solar cells.

Table 1. Parameters for TiO_2, Go and N719 Ruthenium Dye

Material properties	TIO_2	Go	N719 Ruthenium Dye
Thickness(nm)	2000	200	Vary
Bandgap (ev)	3.2	3.25	2.37
Electron affinity(ev)	4.200	1.9	3.9
dielectric permittivity(relative)	10	3	30
CB effective density of states (1/cm^3)	2.000E+17	2.2E+21	2.400E+20
VB effective density of states (1/cm^3)	6.000E+17	1.8E+21	2.500E+20
Electron mobility (cm^3 /Vs)	100	100	5
hole mobility (cm^3 /Vs)	25	300	5
Shallow uniform donor density ND (1/cm^3)	1.000E+17	0	0
Shallow uniform acceptor density ND (1/cm^3)	0	1 E+16	1 E+17

Table 2. Parameters of back and front contacts

Parameters	Back contact	Front contact
Surface recombination velocity of electrons	1.00E+5	1.00E+5
Surface recombination velocity of holes	1.00E+7	1.00E+7
Metal work function(ev)	5.1	4.4

3. RESULTS AND DISCUSSION

3-1 Simulation of TiO_2/N719-dye/Go and TiO_2/Go solar cells

The J-V characteristics and performance of two different types of solar cells, TiO_2/N719-dye/GO (three layers) and TiO2/Go (two layers), have been studied using SCAPS simulations under standard simulated solar light of AM 1.5G (100mW/cm^2). Based on the results in figure 1, the TiO_2/N719-dye/Go solar cell exhibits the best performance with an open circuit voltage (Voc) of 1.02V, short current density (Jsc) of 3.5mA/cm^2, and a maximum output power (P_{max}) of 0.9mW/cm^2. The fill factor of the three-layer solar cells was around 0.67, calculated using equation 1 [16].

$$FF = \frac{I_m V_m}{I_{sc} V_{oc}} = \frac{P_{max}}{I_{sc} V_{oc}} \tag{1}$$

The power conversion efficiency (η) of a solar cell is given by the ratio of the maximum output power (P_{max}) to the power of the incident light (Pin). Mathematically, it can be expressed as:

$$\eta = \frac{P_{max}}{P_{in}} \tag{2}$$

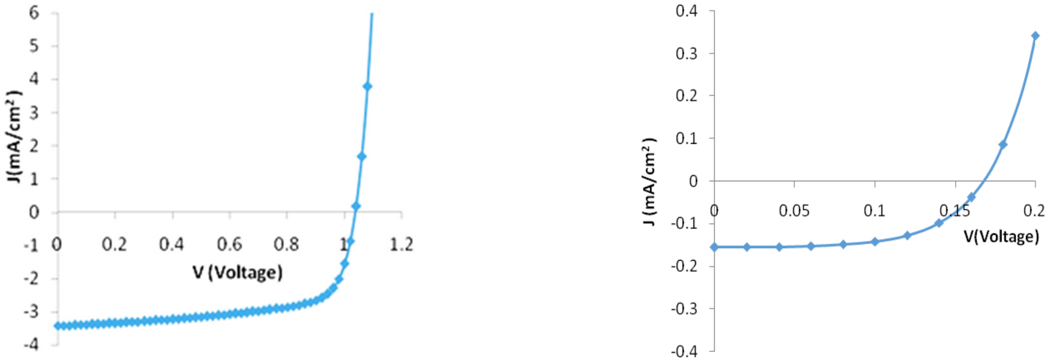
The maximum output power (P_{max}) can be obtained by multiplying the open-circuit voltage (V_{oc}) and the short-circuit current density (Jsc), and then multiplying the result by the fill factor (FF) of the solar cell. Therefore, we can express Pmax as:

$$P_{max} = Voc \times Jsc \times FF \tag{3}$$

Substituting equation (2) into equation (1), we get:

$$\eta = \frac{Voc \times Jsc \times FF}{P_{in}} \tag{4}$$

From equation (4), It is clear that the fill factor (FF) plays a crucial role in determining the power conversion efficiency (η) of a solar cell. A high fill factor indicates that the solar cell is able to convert a higher fraction of the incident light into electrical power, resulting in a higher efficiency. On the other hand, a low fill factor indicates that the solar cell is not able to utilize the incident light efficiently, resulting in a lower efficiency. It's important to note that no additional defects or recombination reactions were introduced in each layer during the simulation.



a

b

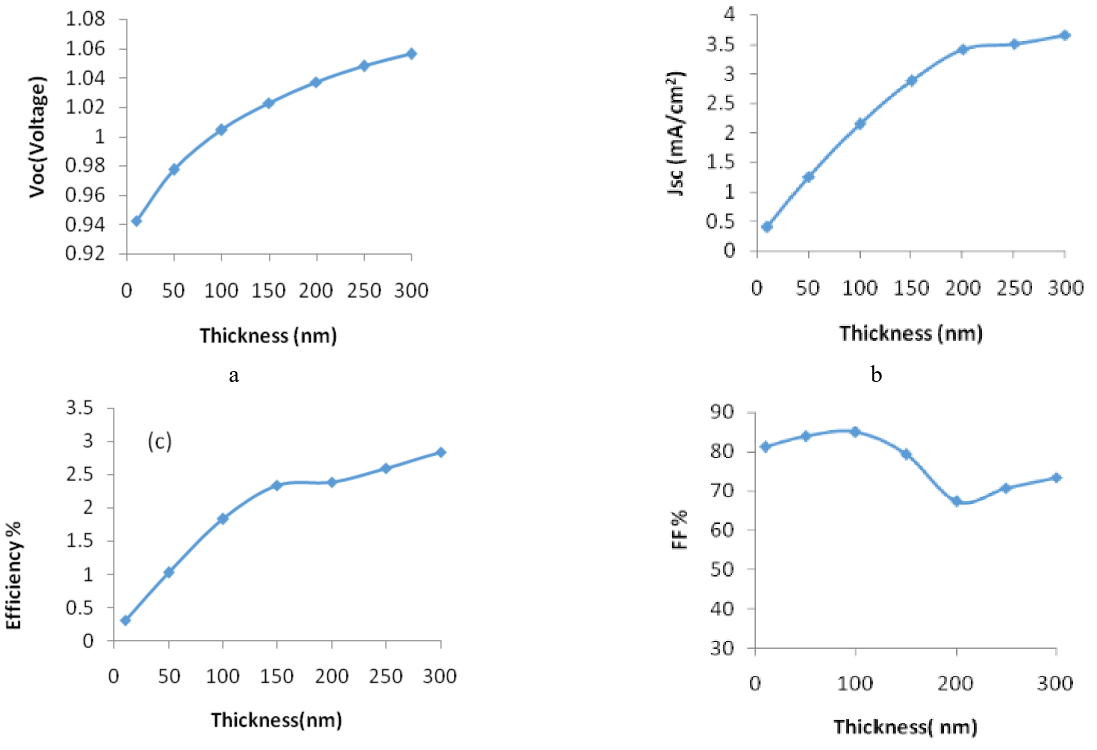
Figure 2. a) J -V characteristics of Go/DYE/TiO_2 solar cell and (b) J -V characteristics of Go /TiO_2 solar cell under illumination

The study found that a three-layer device composed of TiO_2, dye, and Go showed an efficiency of 2.5% based on numerical simulations, which is higher than the reported 0.9% efficiency in recent literature [17]. Further investigated were conducted on three-layer solar cell by varying the thickness of the dye layer and the work function of the back contact and operating temperature, this could provide data on the relationship between these parameters and the efficiency of the solar cells. This data could then be analyzed to identify optimal values for these parameters that result in the highest efficiency. This process of optimizing the design of a solar cell is an important step in improving its performance and could lead to the development of more efficient and cost-effective solar energy technologies.

3-2. Effect of Thickness of N719 dye layer on solar cells

In dye-sensitized solar cells, the thickness of the dye layer plays an important role in the absorption of photons and the separation of photogenerated carriers at the interfaces between the dye layer and the metal oxide layer. The dye layer is responsible for absorbing light and transferring the energy to the metal oxide layer, where it generates electron-hole pairs. Figure 3 shows the dependence of various photovoltaic parameters on the thickness of dye, which was changed in the range of 10-300nm.

Figure 3a specifically shows the variation of V_{oc} with a change in the thickness of the dye layer. It appears that at 10 nm thickness, V_{OC} was initially around 0.94V, but as the thickness of the dye layer increased, V_{OC} also increased to reach 1.06V at 300 nm thickness. According to Figure 3b and c, the short-circuit current (Jsc) and efficiency of the three-layer solar cells increased with an increase in the thickness of the dye layer. At a thickness of 200 nm, the Jsc and efficiency reached approximately 3.5 mA/cm^2 and 2.5%, respectively. However, as the thickness of the dye layer increased beyond 200 nm, the enhancement of Jsc and efficiency became very slow, indicating that there is an optimal thickness range for maximizing these parameters. This behavior can be explained by the fact that an increase in the thickness of the dye layer leads to the absorption of more light by the device, which generates more excitons (electron-hole pairs) that can contribute to the photocurrent. However, beyond a certain thickness, the additional dye molecules may not contribute significantly to the generation of excitons, leading to a plateau in the Jsc and efficiency values. A thinner dye layer may produce lower short-circuit current density and efficiency because of several factors. One of these factors is an increase in the recombination rate near the interfaces between the graphene oxide (GO)/dye and dye/ TiO_2 layers, which can limit the photocurrent generation. Additionally, a thinner dye layer may not absorb enough light, resulting in a lower photocurrent. Furthermore, the thickness of the dye layer should not be larger than the diffusion length of charge carriers, as a thick layer can reduce the short-circuit current density due to an increase in series resistance. In Figure 3d, the behavior of the fill factor was almost constant at the beginning, but it then declines for dye layers thicker than 100 nm, reaching a value of 67 at a thickness of 200 nm. This behavior indicates an increase in the series resistance, which can affect the fill factor. As the thickness of the dye layer increases, the series resistance also increases, leading to a decrease in the fill factor.



a b

c d

Figure 3. Photovoltaic performance parameters at various thickness of dye layer as: (a) Voc, (b) Jsc, (c) efficiency, and (d) FF

3-3. Effect of operating temperature on the performance of N719 dye layer on solar cells

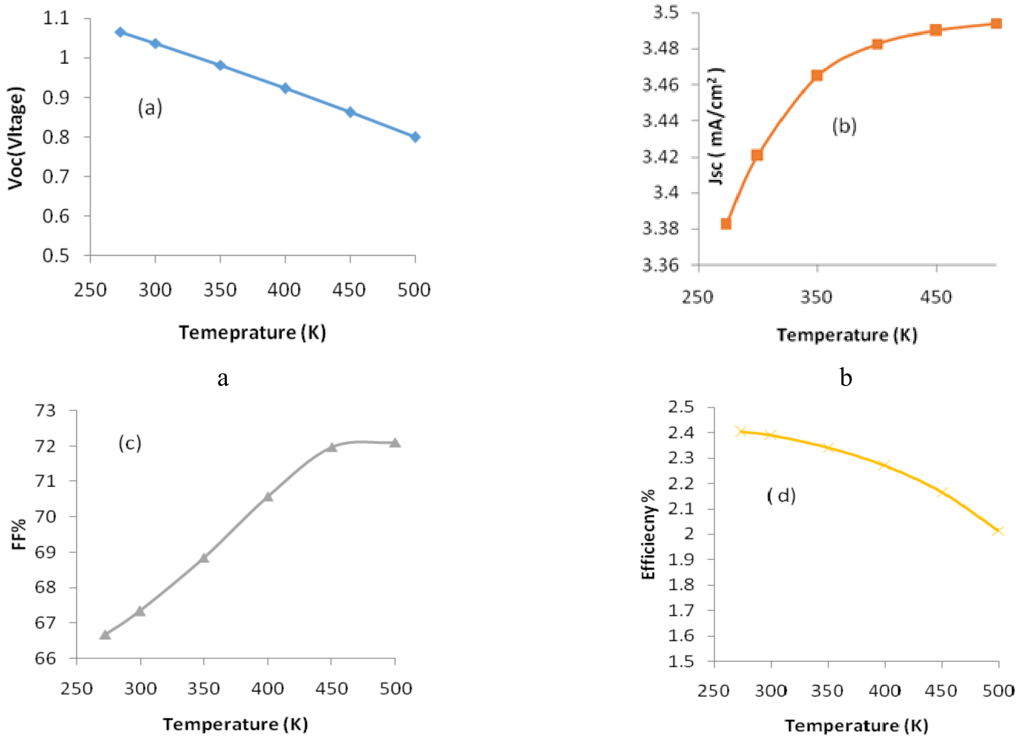
The effect of temperature on the performance of solar cells is a crucial factor to consider for achieving optimal efficiency and durability. This section examines the effect of temperature on the performance of TiO_2/dye/Go solar cell. Figure 4a shows the temperature of solar cells increases, the short circuit current density increases slightly due to improved light absorption and generation of electron and hole pairs. That is attributed to thermal energy breaks some of the bonds between the atoms or molecules in the material, causing the band gap to decrease. This allows electrons to absorb photons with lower energies, which results in improved light absorption and increased generation of electron and hole pairs [18].

As a result, the short circuit current density increases slightly at higher temperatures, reaching 0.35 mA/cm^2 at high temperature. As the temperature of solar cells increases, more electrons and/or hole carriers are generated, leading to an increase in the reverse saturation current density (Jo). According to the Shockley diode equation (4) , there is an inverse relationship between the reverse saturation current density and the open circuit voltage [19].

$$V_{oc} = \frac{nK_B T}{q}\left[\ln(1+\frac{J_{sc}}{J_o}\right]. \tag{5}$$

Where, Voc is the open circuit voltage,A is ideally factor , q is elementary charge, K$_B$ is Boltsman constant , Jo is reverse current.

This means that an increase in Jo will lead to a decrease in the open circuit voltage. Therefore, as the temperature of solar cells increases, the open circuit voltage will decrease, as observed in Figure 4b. The operating temperature of a solar cell can have a significant impact on its power conversion efficiency (Figure 4 c). At higher temperatures, there can be changes in the properties of the semiconductor materials used in the solar cell, which can lead to a decrease in efficiency. This degradation in efficiency is due to changes in the physical and chemical properties of the semiconductor materials used in the solar cells [18,19]. That is attributed to change in the characteristics of semiconductors used in the solar cells. The high temperature causes to change in the electron and hole mobility, carrier concentrations and band gaps of the materials. For example, the band gap of semiconductor become narrow at high temperature which my lead the increase the recombination of electrons and holes while traveling across the region decrease of efficiency output power of the device (Jsc Voc) [18]. The increase in fill factor (FF) of a solar cell from 67% to 72% with increasing temperature up to 450 k is likely due to a reduction in the series resistance within the bulk region of the solar cell. Series resistance is the sum of the resistances within a solar cell that limit the flow of current. As the temperature increases, the resistance of the bulk material of the solar cell decreases. This reduction in resistance can lead to a decrease in the voltage drop across the cell, resulting in an increase in the fill factor.



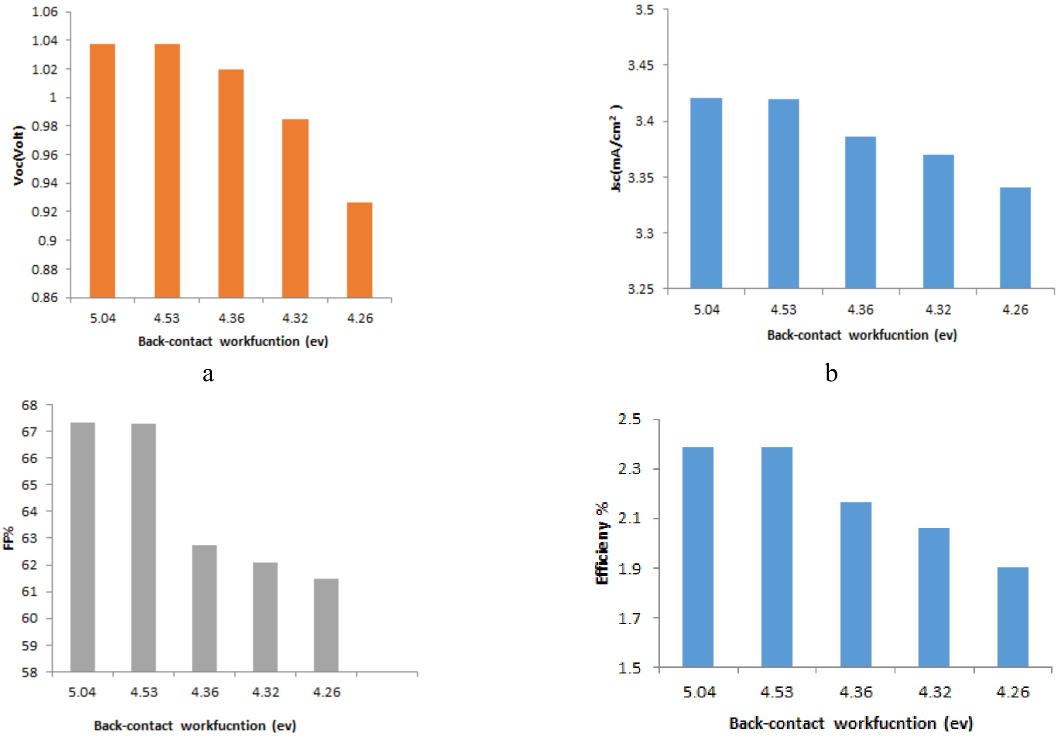
a b

c d

Figure 4. Photovoltaic performance parameters at various thickness of dye layer as: (a) Voc (b) Jsc, (c) efficiency and (d) FF

3.4 Effect of back-contact workfucntion

In solar cells, it is important to optimize the alignment of energy levels of materials and work function of electrodes to ensure efficient charge transfer and minimize energy losses. To achieve this, the energy levels of the materials and electrodes must be aligned properly so that the charge carriers can flow efficiently from one to another without losing energy. It is desirable to have a small energy level offset between the electrodes and the hole transport layer in order to maximize the efficiency of the solar cell. A small offset can facilitate the injection of holes from the hole transport layer into the electrode, leading to efficient charge extraction and high photocurrent. Figure 5 demonstrates the impact of changing the back contact work function of a solar cell using different electrodes. Specifically, the back contact work function is varied from 5.04 ev to 4.26ev, and the electrodes used include nickel, silver, copper, molybdenum, and tungsten. According to the graph, the change in Jsc (short-circuit current density) is minimal, with only a 0.02 mA/cm^2 difference observed between the different electrodes. However, the open-circuit voltage decreases slightly from 1.03 V to 0.95 V. The more significant impact is observed in the efficiency and fill factor parameters, as indicated in Figure 5c and 5d. The efficiency of the solar cell decreases considerably with the change in back contact work function, with the maximum efficiency dropping from approximately 20% to 14%. Similarly, the fill factor parameter also decreases with the change in back contact work function, indicating that the cell's ability to convert light into electricity is reduced.



a b

c d

Figure 5. Photovoltaic performance parameters at various Back-contact workfucntion **(eV)** as: (a) – Voc, (b) – Jsc, (c) – FF, and (d) – efficiency

The performance of solar cells is affected by the type of junction created at the interface between the electrode and HTM (hole transport material), as reported by studies [20]. The efficiency obtained in Ag, MO electrode, and Mo solar cells was low due to the large energy barrier at the interface that impedes the flow of the active layer to the electrode. This barrier is known as a Schottky barrier and arises from the difference in work function between the LUMO (lowest unoccupied molecular orbital) of graphene oxide (5.1 eV) and the work function of Ag and Mo (4.26, 4.36 eV). On the contrary, solar cells with Ni and Cu electrodes show high efficiency because an ohmic contact is formed between graphene oxide and the Ni and Cu electrodes. This is attributed to the small difference between the LUMO of GO and the work function of the electrodes, which facilitates efficient charge transfer and helps to form an ohmic contact.

4. CONCLUSION

The SCAPS-1D simulation was utilized to investigate the impact of several parameters on the performance of TiO_2/N719-dye/GO solar cells. These parameters included the thickness of the dye layer, operating temperature, and work function of the back contact. The simulation results indicated that the Go/N719dye/TiO2 solar cells demonstrated higher Jsc, Voc, and η compared to the Go/TiO2 solar cells. The Jsc increased from 0.17 mA/cm^2 to 1 mA/cm^2, the Voc increased from 0.2 V to 1 V, and the η increased from 0.02% to 2.5%. These enhancements were ascribed to the improved light absorption and charge transport through the interface due to the presence of the dye layer. Furthermore, it was found that the optimal dye layer thickness for achieving high Jsc, Voc, and η was between 200nm and 300nm. However, increasing the dye layer thickness resulted in a decrease in the fill factor. Moreover, the increase in operating temperature had a negative impact on the Voc and η, while slightly enhancing the Jsc. This is due to changes in the electron and hole mobility, carrier concentrations, and band gaps of the materials at high temperatures. The type of electrode used also influences the efficiency of TiO_2/dye/Go solar cells. Ni and Cu electrodes create low resistance at the interface with Go, while Ag and M electrodes create a high barrier that inhibits the flow of charge carriers across it.

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SCAPS ЧИСЛОВИЙ АНАЛІЗ ОБ’ЄМНОГО ГЕТЕРОПЕРЕХОДУ СОНЯЧНОГО ЕЛЕМЕНТУ ОКСИДУ ГРАФЕНУ/TiO_2, СЕНСИБІЛИЗОВАНОГО БАРВНИКОМ РУТЕНІЮ n719

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Твердотільні сенсибілізовані до барвника сонячні елементи (SSDSC) були виготовлені з використанням двох різних металооксидних матеріалів, оксиду графену та оксиду титану, які використовуються як матеріали для транспортування дірок та електронів відповідно. Барвник Рутеній-N719 між матеріалами для транспортування дірок і електронів, діє як шар поглинача у сонячних елементах Go/N719dye/TiO_2. За допомогою моделювання SCAPS-1D було виявлено, що сонячні батареї Go/N719dye/TiO_2 значно покращили продуктивність сонячних елементів порівняно з сонячними елементами Go/TiO_2. Зокрема, струм короткого замикання (Jsc) збільшився з 0,17 мА/см^2 до 1 мА/см^2, напруга холостого ходу (Voc) зросла з 0,2 В до 1 В, а ефективність перетворення потужності (η) зросла з 0,02 % до 2,5 %. Крім того, різноманітні фактори можуть впливати на продуктивність сонячних батарей Go/N719 dye/TiO_2. Було виявлено, що оптимальна товщина барвника для досягнення високої щільності струму короткого замикання, високої ефективності перетворення потужності та високої напруги холостого ходу становить від 200 нм до 300 нм. Крім того, робоча температура сонячних батарей також впливає на їх продуктивність. Підвищення робочої температури негативно впливає на напругу холостого ходу та ефективність перетворення потужності елементів, у той час як щільність струму короткого замикання трохи підвищується. Нарешті, ефективність сонячної батареї може залежати від типу металу, який використовується для електрода, і типу напівпровідникового матеріалу, який використовується в комірці. У сонячних елементах з Ni та Cu електродами омічні контакти забезпечують ефективну передачу електронів, тоді як бар’єри Шотткі можуть перешкоджати потоку електронів і знижувати ефективність сонячних елементів із електродами Mo та Ag.

Ключові слова: *SCAPS; оксид графену; робоча температура; товщина; робоча функція; параметри сонячних елементів*