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SCAPS NUMERICAL ANALYSIS OF GRAPHENE OXIDE/ZIRCONIUM DISULFIDE SOLAR CELLS

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This work studies the performance of solar cells composed of two different materials, graphene oxide (Go, hole transport material) and zirconium disulfide (ZrS_2, electron transport materials) using the SCAPS -1D simulation. It has been found that Go/ZrS_2 solar cells show better performance with high short circuit current, J_{sc}, of 38 mA/cm^2 and the power conversion efficiency, η, of 17% compared with other solar cells based on graphene oxide and perovskite materials. Additionally, the short circuit current density decreases from 38 mA/cm^2 to 22 mA/cm^2 when the energy gap of ZrS^2 increases from 1.2 eV to 17 eV. The increasing the operating temperature and the work function of back contact also led to decrease the open circuit voltage and power conversion efficiency of the cells, while the short circuit current density was slightly enhanced. That is attributed to changes in the electrical properties of Go and ZrS_2 layers, including their charge carrier mobility and characteristics of the interfacial layers.
Keywords: *SCAPS-1D simulation; Solar cells; Work function; Interfacial layers; Operating temperature*
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1. INTRODUCTION

There have been significant research and development efforts focused on finding alternatives to fossil fuels for powering factories and industrial development [1]. The primary reasons for seeking alternatives to fossil fuels are the environmental concerns associated with their usage, including greenhouse gas emissions, air pollution, and their contribution to climate change [2]. One of these alternatives is solar energy which is friendly to the environment and available to varying extents also around the Earth [3]. Silicon solar cells have been the most widely used photovoltaic technology due to their high efficiency and relatively low cost. Silicon semiconductors are typically rigid and brittle, making them unsuitable for certain applications that require flexibility, bendability, and require a high power-per-weight ratio [3,4]. These later features have been achieved using organic materials to fabricate flexible solar cells [5,6]. However, organic solar cells have not produced high enough efficiencies and low stability, and low strength to compete with traditional silicon-based solar cells in commercial applications [5].

The disadvantages of silicon and organic materials-based solar cells led to the use of transition metal dichalcogenides (TMDCs) as n-type semiconductor for fabricating solar cells [7]. Particularly zirconium disulfide (ZrS_2) received significant attention due to its potential as a candidate for various applications, including solar cells [7,8]. This material is a two-dimensional (2D) transition metal disulfide and synthesized as thin film for application in flexible transparent devices. Various growth techniques can be employed to achieve tun ability of bandgap energy, electronic, and optical properties for ZrS_2 thin films such as Chemical Vapor Deposition (CVD) and Atomic Layer Deposition (ALD) [8]. The second part of solar cells should be a p-type semiconductor to create a junction at the interface in solar cells such as graphene oxide (GO) [9]. Go has been used widely as a hole transport material and a good candidate to replace organic hole transport layer in solar cells. That is attributed to its bandgap energy (3.5 eV), excellent transparency, low production cost, large-scale production capability and good dispensability in many solvents and high hole mobility. 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 in Belgium. The main purpose of SCAPS-1D is to simulate and evaluate the performance of semiconductor-based solar cells, particularly their electrical characteristics in the dark and light [10-12]. In the beginning, the SCAPS was conducted to simulate the performance of solar cells whose components are $CuInSe_2$ and the CdTe family [11]. Also, it has been used for different types of materials such as crystalline solar cells (Si and GaAs family) and amorphous cells (a-Si and microporous Si) [13]. The SCAPS-1D solves the essential semiconductor equations such as the Poisson equation (1) and the continuity equations for electrons and holes (2,3) [13]. These equations are fundamental in understanding the behaviour and performance of solar cells. The equations are given below:

$$\frac{\dot{d}^2\psi}{dx^2}+\frac{q}{\varepsilon}\left[p(x)-n(x)+N_D-N_A+\rho_p-\rho_n\right]=0\,, \tag{1}$$

$$\frac{1}{q}\frac{\dot{d}J_P}{dx}=G_{op}-R(x)\,, \tag{2}$$

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$$\frac{1}{q}\frac{\dot{d}J_n}{dx} = -G_{op} + R(x)\,. \tag{3}$$

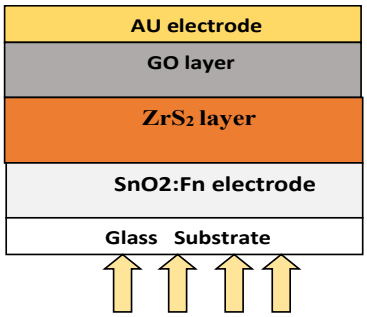

Figure 1. Schematic representation of the solar cell structure

Where ε is the dielectric constant, q is the electron charge, N_A and N_D are ionized acceptors and donor density, Ψ is the electrostatic potential, Jp is current density due to hole, Jn is current density due to electron, G_{op} is the carrier generation rate, R is the total recombination rate, p is free hole density, n is the free electron density, ρ_p, and ρ_n are the hole and electron distribution. The following drift-diffusion equations (2) and (3) represent the holes and electrons carrier transport properties of the semiconducting material. In this work, the SCAPS simulator has been used to study the dependence of parameters of solar cells on the operating temperature and the work function of back contact and energy gap of ZrS_2. These parameters are power conversion efficiency (η), short circuit current density (J_{sc}), fill factor (FF) extracted by drawing the current density versus voltage of solar cells under different conditions. The proposed solar cell in the work is composed of zirconium disulfide (ZrS_2) and Graphene oxide (Go) and front – contact (fluorine-doped tin dioxide, SnO_2;Fn) and back-contact (Gold, Au). Figure 1 shows schematic diagrams of SnO_2; Fn/ZrS_2/Au solar cells.

From previous literatures (8-9, 14-18) Table 1 and 2 present the input parameters used in SCAPS simulators for studying the performance of solar cells.

Table 1. Parameters for ZrS_2 and Go materials

Material properties	Zirconium disulfide (ZrS_2)	Graphene Oxide (Go)
Thickness (μm)	1	0.200
Bandgap (eV)	Varying (1.2 to 1.7)	3.25
Electron affinity(eV)	4.7	1.9
Dielectric permittivity(relative)	16.4	3
CB effective density of states (1/cm^3)	2.2E+19	2.2E+21
VB effective density of states (1/cm^3)	1.8E+19	1.8E+21
Electron mobility (cm^3/Vs)	300	100
Hole mobility (cm^3/Vs)	30	300
Shallow uniform donor density ND (1/cm^3)	1.000E+19	0
Shallow uniform acceptor density ND (1/cm^3)	0	1 E+16

Table 2. Parameters of back and front contacts

Parameters	Back- contact Au	Front- contact SnO_2;Fn
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

2. RESULTS AND DISCUSSION

2.1. The parameters of SnO_2:Fn/ZrS_2/Gu/Au solar cells under illumination

Figure 2 shows the Current-Voltage (J–V) characteristics of SnO_2:Fn/ZrS_2/GO/AU solar cells using SCAPS simulations under the standard simulated solar light of AM 1.5G (100 mW/cm^{-2}) at room temperature. As seen, the device produces a high short-circuit current density of 38 mA/cm^2, open circuit voltage of 0.6 V and a Fill factor of 80 %. This structure shows better performance with high power conversion efficacy of 17 % compared with other solar cells based on graphene oxide and perovskite materials [19]. These results were obtained when the energy gap of ZrS_2 and Go were 1.2 eV and 3.25 eV.

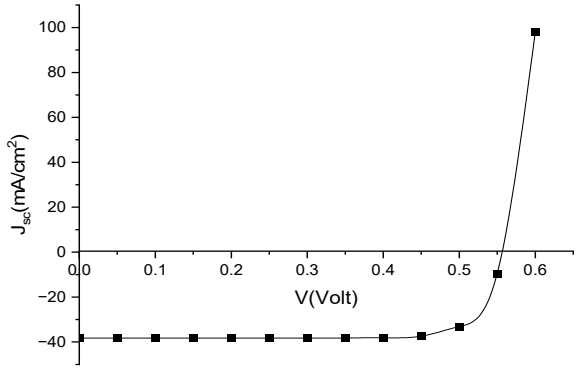

Figure 2. J -V characteristics of SnO_2:Fn/ZrS_2 /GO/ Au solar cells under illumination

2.2. Effect of energy gap of SZr_2 layer on parameters of SnO_2: Fn /ZrS_2/Go/Au solar cells

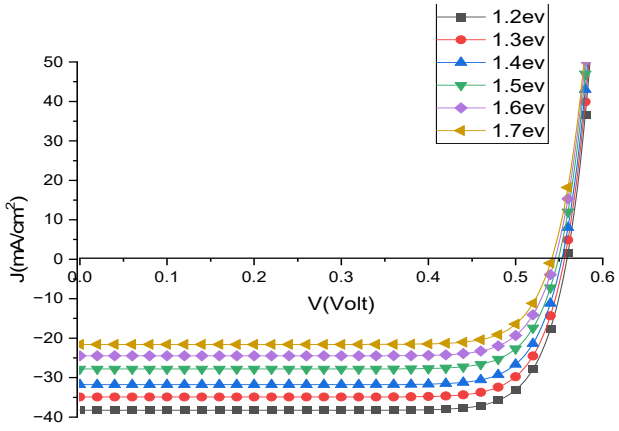

Figure 3. J-V characteristics of SnO_2:Fn/ZrS_2/Go/Au solar cells as function of energy gap of SZr_2 layer

Figure 3 show that the short circuit current density (J_{sc}) and open circuit voltage (V_{oc}) decreases from 38 mA/cm^2 to 22 mA/cm^2 and 5.5 V to 5.4 V as the energy gap of SZr_2 change from 1.2 eV to 1.7 eV receptively. The behavior of power conversion efficiency (η) is similar to that of J_{sc}, with a general decreasing from 17% to 9% when the energy gap of ZrS_2 increase from 1.2 eV to 1.7 eV. That is attributed to many reasons such as 1) the absorbed photons may have less energy to create electron-hole pairs, potentially leading to a lower voltage output, 2) limit the number of electron-hole pairs that can be generated by absorbing photons which causes to decrease in the current output of the solar cell [8]. On the other hand, V_{oc} (open-circuit voltage) decrease from 0.55 V to 0.54 V while FF (fill factor) values of simulated devices remain almost constant with the increase of bandgap of the ZrS_2 layer.

2.3. Effect of operation temperature on parameters of SnO_2: Fn /ZrS_2/Go/Au solar cells

As known, the ambient temperature plays an important role in the operation of solar cells because solar cells are more commonly used outdoors due to their reliance on sunlight. Here the effect of temperature on the parameters of solar cells has been investigated under light conditions presented.

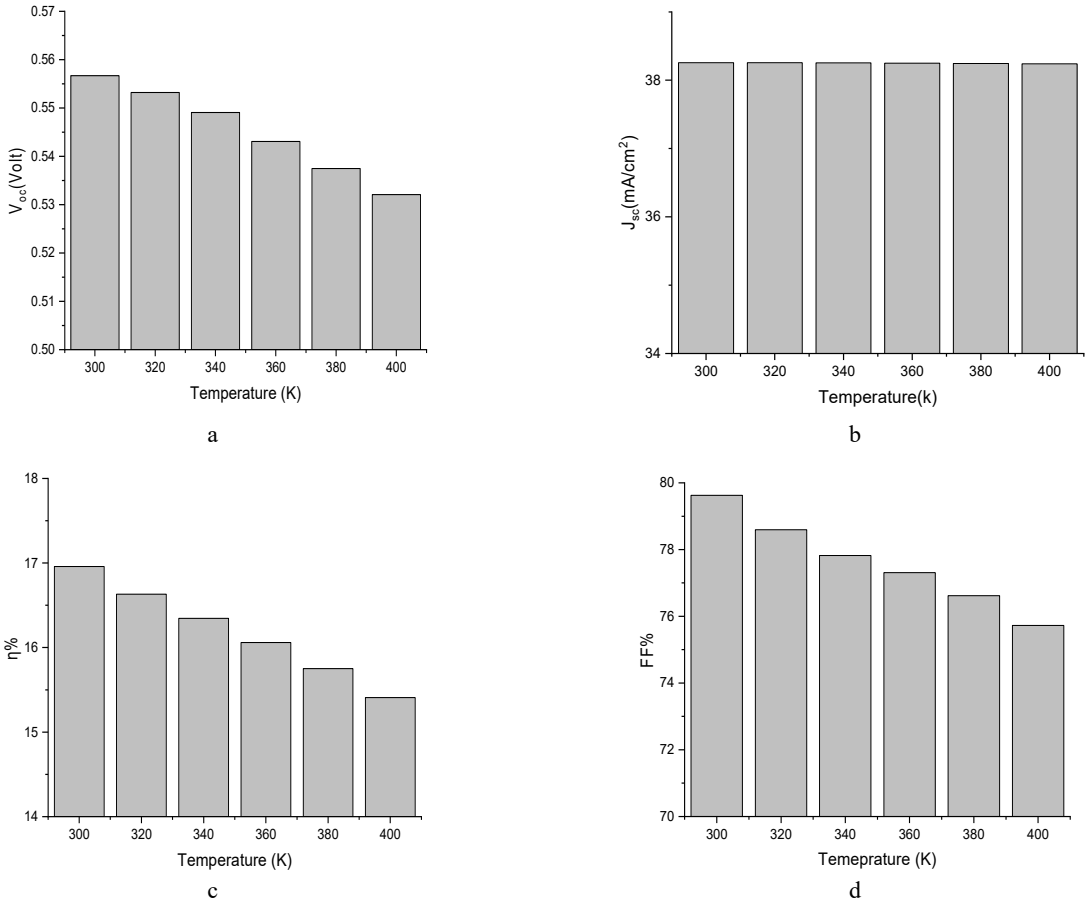

Figure 4. Variation of solar cells parameters (Voc, Jsc, η and FF) with change in temperature

Figure 4 shows the variation of open circuit voltage (V_{oc}), short circuit current density (J_{sc}), Fill factor (FF%), and power conversion efficiency (η%) with changing temperature from 300k to 400k. As seen the parameters of SnO_2:Fn/ZrS_2/GO/AU solar cells decline steadily as the temperature increase. When the temperature of solar cells increases, more electron-hole pairs are generated due to the increased thermal energy and lead to an increase in the reverse saturation current density (J_o). This additional carrier generation can lower the voltage across the solar cell, causing a decrease in the open circuit voltage (see Figure 4a). That agrees with the Shockley diode equation which presents an

inverse relationship between the reverse saturation current density (J_o) and the open circuit voltage (V_{oc}) in solar cells [16,20]

$$V_{oc} = \frac{nK_BT}{q}\left[\ln(1+\frac{J_{sc}}{J_o}\right]. \quad (4)$$

Where V_{oc} is the open circuit voltage, A is the ideal factor, q is the elementary charge, K_B is the Boltzmann constant, Jo is the reverse current.

At higher temperatures, there can be changes in the characteristics of the materials used and reduce the efficiency and fill factor of solar cells (see Figure 4-c and 4-d). This degradation is due to changes in the physical and chemical properties of the semiconductor materials used in solar cells [16, 21]. High temperature breaks some of the bonds between the atoms or molecules in the solar cell. That cause to decrease the energy gap of materials, change in the mobility and concentrations of charge carriers. For example, the energy gap of the semiconductor becomes narrow at a high temperature which may lead to an increase in the recombination of electrons and holes while travelling across the region decrease of efficiency output power of the device and Fill factor [20]. Finally, there was a slight decrease in short circuit current density since the charges separation processing at the interface was also reduced (see Figure 4 b).

2.4 Effect of back-contact work function

In solar cells, the alignment of energy levels in materials used for solar cells is a crucial aspect of achieving efficient charge transfer and minimizing energy losses. This can involve selecting appropriate materials with suitable energy levels, modifying the device architecture, or using interfacial layers to adjust the energy level alignment [22]. Figure 5 shows parameters of SnO_2:Fn/ZrS_2 /Go/ AU solar cells versus different back- contact work function.

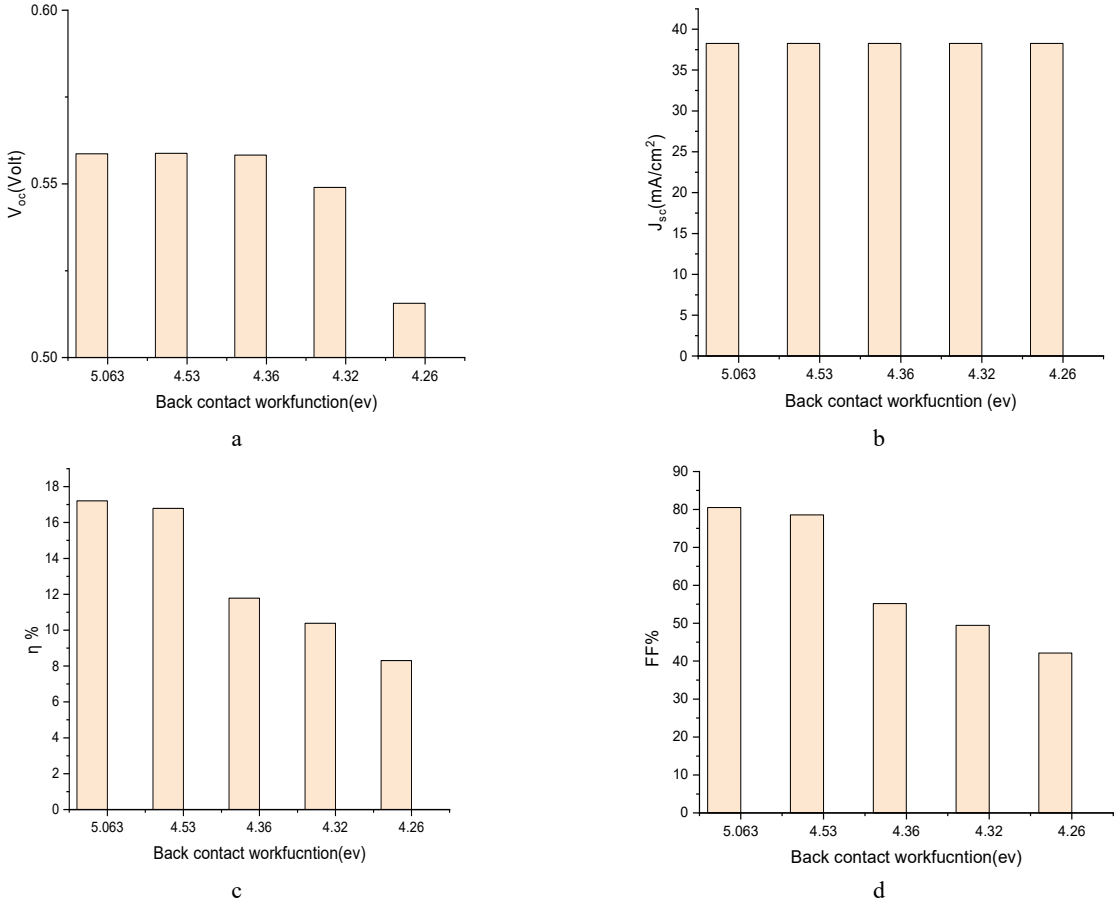

Figure 5. Photovoltaic performance parameters at various Back-contact work function (eV) as:
(a) Voc, (b) Jsc, (c) η, and (d) FF

They are made of (nickel (Ni), φ=5.03 eV, silver (Ag, φ=4.26 eV), copper (Cu, φ=4.53 eV), molybdenum (Mo, φ=4.36 eV) and tungsten (W, φ=4.32 eV). The low efficiency in Ag, Mo electrode, and Mo solar cells is attributed to the presence of a Schottky barrier at the interface between graphene oxide) and the Ag/Mo electrodes. This barrier arises from the difference in work function between these materials. That cause to hinders the movement of hole charge carriers at the interface leading to a reduction in the open-circuit voltage and fill factor. On the other hand, Ni and Cu electrode

solar cells produced the high-efficiency and open circuit voltage and fill factor because of a small energy difference between the LUMO of Go and the work function of the electrodes. That facilitates efficient charge transfer by achieving an ohmic contact and improving the overall performance of the solar cell.

3. CONCLUSION

The Go/ZrS_2 solar cells exhibit high performance compared to other solar cells based on graphene oxide and perovskite materials. The Go/ZrS_2 solar cells achieve a high short circuit current (Jsc) of 38 mA/cm², and a power conversion efficiency (η) of 17%. This indicates that they have ability to generate a significant amount of current and convert a considerable portion of sunlight into electricity. However, the study also highlights that certain factors negatively affect the performance of the solar cells. An increase in operating temperature and energy bandgap of ZrS_2, as well as changes in the work function of the back contact material, lead to a reduction in parameters of solar cells. These effects are attributed to changes in the electrical properties of the Go and ZrS_2 layers such as charge carriers mobility and interfacial layer properties.

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ЧИСЛОВИЙ SCAPS АНАЛІЗ СОНЯЧНИХ ЕЛЕМЕНТІВ НА ОКСИДІ ГРАФЕНУ/ДИСУЛЬФІДУ ЦИРКОНІЮ

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Ця робота вивчає продуктивність сонячних елементів, що складаються з двох різних матеріалів, оксиду графену (Go, матеріал для транспортування дірок) і дисульфіду цирконію (ZrS_2, матеріали для транспортування електронів) за допомогою моделювання SCAPS-1D. Було виявлено, що сонячні батареї Go/ ZrS_2 демонструють кращу продуктивність із високим струмом короткого замикання Jsc 38 мА/см^2 і ефективністю перетворення потужності η 17% порівняно з іншими сонячними елементами на основі оксиду графену та перовскітних матеріалів. Крім того, щільність струму короткого замикання зменшується з 38 мА/см^2 до 22 мА/см^2, коли енергетичний зазор ZrS_2 збільшується з 1,2 еВ до 17 еВ. Підвищення робочої температури та робочої функції зворотного контакту також призвело до зниження напруги холостого ходу та ефективності перетворення потужності елементів, у той час як щільність струму короткого замикання дещо збільшилася. Це пояснюється зміною електричних властивостей шарів Go і ZrS_2, включаючи їх рухливість носіїв заряду та характеристики міжфазних шарів.

Ключові слова: *моделювання SCAPS-1D; сонячні елементи; робота виходу; міжфазні шари; робоча температура*