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Analysis of nickel oxide as a counter electrode for dye-sensitized solar cells using OghmaNano software

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ABSTRACT

Dye-sensitized solar cells (DSSCs), a promising green technology, convert solar energy into electricity more cost-effectively than traditional solar cells. While platinum (Pt) is commonly used in DSSCs, its high cost and toxicity limit practical applications. Recent research aims to develop low-cost counter electrodes with high efficiency. Nickel oxide (NiO), a p-type semiconductor with a wide bandgap, good transmittance, and suitable work function, emerges as a potential alternative for counter electrode of DSSCs. In this work, DSSCs with NiO of thicknesses varying from 100 nm to 1000 nm were simulated to determine its influence on photovoltaic performance using OghmaNano software. The structure of simulated solar cells consists of NiO as counter electrode, zinc oxide (ZnO) as photoanode, N719 as dyes, electrolyte as charge carrier transport, and fluorine-doped tin oxide (FTO) as a contact layer. There are five data of NiO used as an active layer. From the simulation results, NiO-doped gold exhibits the highest power conversion efficiency (PCE) of 15.95% at a thickness of 700 nm, while pure NiO shows the lowest PCE with 4.53% at a thickness of 600 nm. These results have demonstrated that NiO can replace Pt as a counter electrode for DSSCs and doping plays a vital role in increasing efficiency.

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1. INTRODUCTION

There are many potentials uses for dye-sensitized solar cells (DSSC); thus, it has been the subject of intense study over the past decade. These uses vary from renewable energy and flexibility to alternative energy sources. Within inorganic DSSCs, the generation of electrical current can be summarized into 4 key steps: i) Excitons are created when light photons are absorbed; ii) Then, excitons diffuse at the donor-acceptor interface; iii) Subsequently, the exciton dissociates into charge carriers while relaxing with the help of charge carriers; and iv) All electrons and holes flow to their respective cathode and anode contacts where the process then repeats [1]-[3]. In DSSC, the counter electrode is an important layer as for example, in the redox electrolyte formed of iodine and iodide, the counter electrode's role is to transfer electrons from an external circuit to the tri-iodide and iodine [4]. (Pt) is typically used as a catalyst because of its high conductivity and

electrocute-lytic properties, but it comes at a high cost when used on a large scale [5]. The RF magnetron co-sputtering method also prepared metal oxide bi-phase counter electrodes (Pt/NiO [6], [7] and Pt/TiO2 [7]). However, high-efficiency Pt/NiO (or Pt/TiO2) bi-phase counter electrodes require costly vacuum technology and precise process control. Currently, many researchers are focusing on p-type oxide semiconductors as hole transport layers or counter electrodes. This is because tandem photovoltaic devices combine p-type oxide cathodes with n-type oxide anodes, which can increase efficiency and decrease the cost of solar harvesting systems [8].

The primary concern regarding platinum pertains to its elevated cost, which renders it unfeasible for practical applications in real-world contexts. Therefore, this study introduces a novel solution for the counter electrode by employing NiO as a cost-effective substitute. The objective of this substitution is to improve the efficiency of dye-sensitized solar cells (DSSCs) by using the advantageous properties of NiO, such as its cost-effective raw materials, excellent durability, and strong chemical stability, together with its promising electrical and optical characteristics [9]-[11]. Furthermore, NiO is a p-type, high-work function semiconductor with a bandgap of 3.6-4.0 eV [12]-[14]. NiO has previously been employed as an HTL in several prior studies to improve the performance of CdTe, organic, DSSC, and perovskite solar cells [14]-[17]. In addition, an interfacial layer (or HTL) is often inserted between the ITO anode and the p-type layers to collect the generated holes and prevent minority carrier injection (electrons) [18]. However, NiO was used for DSSC counter electrodes. Guai *et al.* [19] demonstrated a DSSC with a sulfur-doped NiO counter electrode that achieved a power conversion efficiency (PCE) of 5.04%. Then, Okumura *et al.* [20] achieved a PCE of 5.11% with a DSSC using NiO hybridized carbon film as the cathode. Wang *et al.* [21] achieved the highest PCE of 7.58% for NiO/PEDOT: PSS as the counter electrode. Maitra *et al.* [22] showed that using nickel-doped molybdenum oxide for the counter electrodes increased efficiency to 4.17%. However, DSSC counter electrodes made of NiO and conductive polymers have not been studied yet till today.

This paper simulates DSSCs using NiO with varying thickness as the counter electrode using OghmaNano software. The DSSCs with varying NiO thickness as a counter electrode were simulated using OghmaNano software to investigate the potential of the materials. The OghmaNano is a general-purpose tool for simulating optoelectronic and photovoltaic devices. This software uses finite differences algorithms to solve the drift-diffusion equations for electrons and holes within devices. The DSSCs internal structure consists of FTO/ZnO&N719/Electrolyte/NiO/FTO. The electrical stimulation only reaches the active layer, whereas, in this simulation, the active layer only focuses on NiO [23]-[29]. The thickness of NiO was varied from 100 nm to 1000 nm to deter-mine the optimal thickness to achieving the best the power conversion efficiency (PCE), open circuit voltage (Voc), short circuit current density (Jsc), and fill factor. The OghmaNano results that an optimal layer NiO is needed to maximize the PCE of the DSSC.

2. METHOD

2.1. OghmaNano simulation software

The OghmaNano simulation software is a general-purpose tool for simulating optoelectronics and photovoltaic devices based on a drift-diffusion base. The OghmaNano developed by Dr. Roderick Mackenzie of the University of Nottingham simulates several thin-film devices using drift-diffusion equations and other electrical and optical models. Organic LEDs and perovskite solar cells are examples of thin film technologies al-ready integrated into the system. This work uses this model to simulate the electrical and optical characteristics of the active layer and is unique among similar pro-grammes in that it gives non-experts the ability to create their own thin film devices from scratch. The software can simulate various phenomena, including JV curves, impedance spectroscopy, and ray tracing. The I-V and J-V graphs are displayed using simulation data to demonstrate the pattern of electron density when a voltage is ap-plied to the simulated device. The significant aspects affecting its performance can be investigated to maximize the efficiency of organic solar cells in converting light to electricity. The OghmaNano programmed simulates various layer thicknesses of dye-sensitized solar cells and photons absorbed by the solar cells. The software manual contains a more detailed description of model.

2.2. Electrical model

The electrical simulation consists of 5 distinct layers. The layers are FTO/ZnO&N719/Electrolyte /NiO/FTO. OghmaNano simulated this dye-sensitized solar cell at various active layer thicknesses. Figure 1 illustrates all the layers in detail. The electrical stimulation only reaches the device's active layer, whereas the thickness only focuses on NiO in this simulation. As a result, the fill factor (FF) can be calculated using (1), where Jsc is located at the curve's simulation, and Voc is the maximum out-put voltage. The PCE (η) is given by (2), where Pin denotes the light's power density and Pout indicates the electric power produced by the bulk heterojunction solar device at its highest power point [30].

$$FF = \frac{V_{max}J_{max}}{V_{oc}J_{sc}} \quad (1)$$

$$\eta = \frac{P_{out}}{P_{in}} = \frac{FF*V_{max}J_{max}}{P_{in}} \quad (2)$$

In OghmaNano material databases, the data for NiO, ZnO&N719, and the electrolyte are not provided. Therefore, five data (absorption and refractive index) for NiO from the previous research [23]- [34] were taken and used as an active layer to compare the (PCE). Since the data for the refractive index ZnO with N719 is unavailable, the refractive index from ZnO was used instead [35], [36]. The absorption coefficient (α) was determined using the Beer-Lambert relationship as stated in (3), where A is the absorbance and t is the thickness of the film [37]. The unit of thickness must be in meters to obtain α.

$$\alpha = 2.303A/t \quad (3)$$

Figure 1 shows the layer of the solar cells where fluorine-doped tin oxide (FTO) is the contact layer. FTO is a practical, transparent layer that absorbs UV light and transmits electrons [38]. The thickness of the active layer is critical in a solar cell, where the NiO layer is the material layer used for converting photons into electrons and holes [18].

Table 1 shows the layer thickness and type of layer for each layer of the simulated DSSCs. To study the effect of different types of NiO (NiO doped with La (1) and (2), NiO doped with gold, Co-doped with NiO, and NiO pure) as counter electrodes in DSSC, all layers were fixed at 100 nm. The thickness of the counter electrode was varied from 100 nm to 1000 nm with 100 nm step.

Table 2 shows the electrical parameters changed for layer ZnO&dye, electrolyte, and NiO. All the parameters were extracted from data in literature [39]-[41]. Since OghmaNano software cannot simulate the widest bandgap, the layer of ZnO&dye and electrolyte were also set as an active layer, but only the thickness of NiO was varied. Hence, the large bandgap makes the minority carriers go to zero. Due to the large band gap of ZnO&dye, the minority carrier concentration is neglected within the simulations.

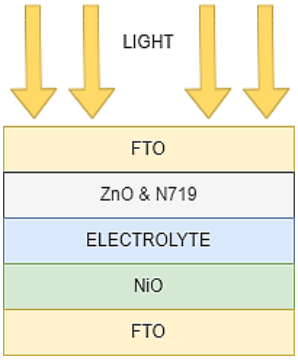


Figure 1. Schematic representation of the simulated DSSC

Table 1. Layer editor in OghmaNano simulation

Layer name	Thickness	Material	Layer Type
FTO	10^{-7}	FTO	Contact
ZnO&Dye	10^{-7}	ZnO&N719	Active layer
Electrolyte	10^{-7}	Electrolyte	Active layer
NiO	10^{-7}–100^{-7}	NiO	Active layer
FTO	10^{-7}	FTO	Contact

Table 2. Electrical parameters used in OghmaNano simulation

Parameter	ZnO&Dye	Electrolyte	NiO
Electron mobility ($m^2v^{-1}s^{-1}$)	0.01 [40]	10-5 [41]	2.8e-05 [42]
Hole mobility ($m^2v^{-1}s^{-1}$)	0.0025 [40]	10-5 [41]	2.8e-05 [42]
Relative permittivity (au)	9 [40]	3.5 [41]	11.7 [38]
Number of traps (bands)	0	0	0
Electron affinity (eV)	3.9 [43]	3.79 [41]	1.64 [42]
Bandgap (eV)	2.37 [43]	1.6 [41]	3.8 [42]

3. RESULTS AND DISCUSSION

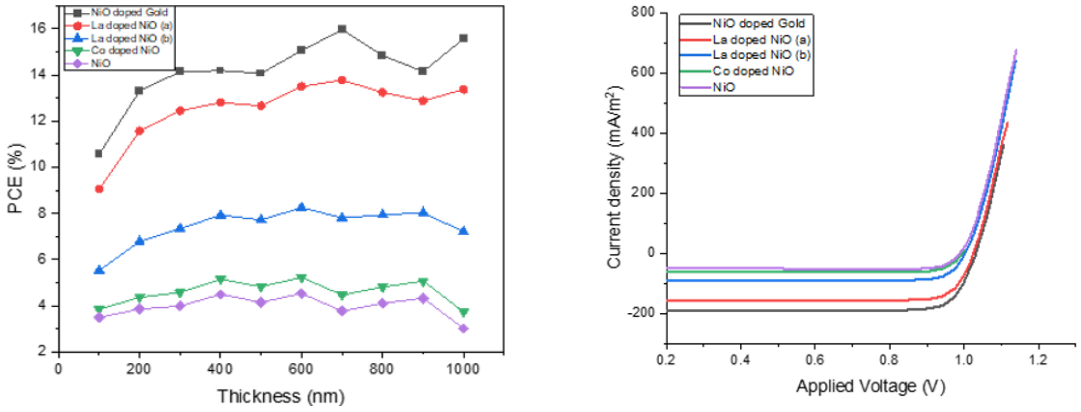
In this section, the research findings will be presented and a comprehensive discussion will be provided. The findings of this study are effectively communicated by employing various visual aids such as figures, graphs, tables, and other graphical representations [42], [43]. These visual aids are strategically utilized to improve the reader's understanding and interpretation of the results. The present discussion has been structured into various sub-sections in order to facilitate a comprehensive examination of the research findings, their implications, and any potential limitations that may arise.

3.1. Electrical simulation

This section discusses the results obtained from the simulation using OghmaNano software of dye-sensitized solar cells using NiO as a counter electrode. The simulation results were divided into the electrical and optical simulations. Different types of NiO, which are NiO doped with La (1) and (2) [44]-[46], NiO doped with gold, Co-doped with NiO, and pure NiO, were used in the simulation to observe how the different composition of the NiO layer influences the PCE, Voc, Jsc, and fill factor. As well as this, the impact of different thicknesses of NiO on the performance of DSSC was also investigated.

The data in Figure 2(a) show the effect of different thicknesses on the performance of various types of NiO on the PCE. As can be observed in Figure 2(a), NiO-doped gold has the highest PCE with 15.95%, followed with NiO doped La (1) at 13.77%, NiO-doped La (2) at 8.26%, Co-doped NiO at 5.23%, and lastly, pure NiO with 4.53%. In several earlier research publications, NiO has been employed as a high-temperature layer (HTL) to improve the performance of CdTe, organic, and perovskite solar cells [40]-[47].

The data in Figure 2(b) shows the current density, J as a function of applied voltage, V for DSSCs with the optimized thickness of the counter electrode. Table 3 summarizes the optimized parameters of V_{oc}, J_{sc}, fill factor, and PCE effect for all DSSCs with different NiO types. As can be seen from the table, all solar cells have high open-circuit voltages (V_{oc}) greater than 0.85 V. The optimized thickness of the counter electrode is around 600 and 700 nm. Gold and La-doped NiO counter electrodes exhibit relatively higher efficiency than Co-doped and pure NiO. These results agree with the experimental results reported where Gold-doped NiO [26]. The highest PCE is gold-doped NiO with 15.95% at 600 nm and lowest PCE is pure NiO, with 4.53% at 700 nm.



(a) (b)

Figure 2. The result of PCE: (a) effect of NiO layer thickness on PCE and (b) J-V characteristic curve at maximum efficiency point

Table 3. The values of Voc, Jsc, FF, and PCE for the NiO

Material	Thickness	Jsc (mA/m2)	Voc (V)	FF (%)	η (%)
Pure NiO	600	-52.808	0.987	0.869	4.533
Lanthanum-doped NiO (La: Nio) (a)	700	-160.72	01.02	0.837	13.77
Lanthanum-doped NiO (La: Nio) (b)	600	-97.54	1.003	0.844	8.2571
Gold-doped NiO (Gold:NiO)	700	-194.56	1.027	0.836	15.95

3.2. Optical simulation

The same device structure of dye-sensitized solar cell: FTO/Zno&dye/electrolyte/NiO/FTO were used for the optical simulation by OghmaNano software to investigate the generation rate and absorbed photon

distribution with the DSSC. The highest PCE and the lowest PCE were compared in the optical simulation. Figure 3(a) show the generation rate profiles of gold doped NiO and Figure 3(b) show the pure NiO as an active layer at the optimized thickness of 700 and 600 nm, respectively. It is evident that the generation rate of gold-doped NiO DSSSC is higher compared to the pure NiO DSSC. Interestingly, the generation also occurs at the gold doped NiO interface.

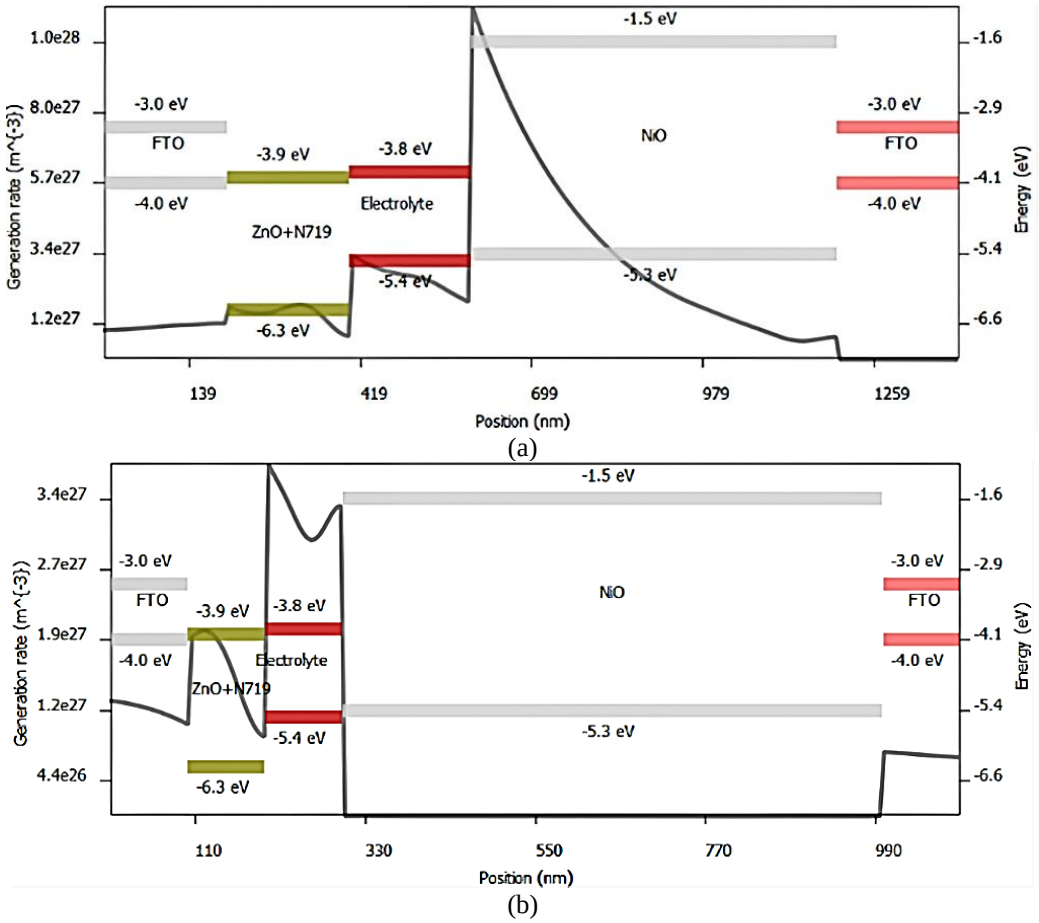


Figure 3. Generation rate profiles of (a) gold:NiO and (b) pure NiO as an active layer at the optimized thickness of 700 mm and 600 mm, respectively

Figure 4(a) represents the absorbed photon distribution of NiO-doped gold at a thickness of 700 nm, corresponding to the maximum value of PCE. In the DSSC with a ZnO&dye thickness of 100 nm, the distribution of the absorbed photon is close to the electrodes. If photon energy exceeds the active layer's bandgap, charge carrier generation and collection potential increase, resulting in a higher fill factor. In a cell with an active area of 700 nm, most absorbed photons have wavelengths ranging from 300 nm to 500 nm. Since photons with longer wavelengths cannot bridge the bandgap, many absorbed photons are required to achieve optimal power conversion efficiency.

As we can see from Figure 4(b), this finding reveals that increasing active layer thickness enhances photon absorption in DSSC, while decreasing the PCE as the in-creased active layer thickness increases photon absorption and excitation, increasing the electron and hole density The greater thickness of the active layer facilitates the extended movement of excitons from their generation point to eventual dissipation. However, within this denser structure, the risk of recombination is heightened due to the restricted mobility of ions, electrons, and holes. Consequently, it is imperative to strike a delicate equilibrium between these contrasting effects. The findings from our simulations indicate that augmenting the thickness of NiO contributes to an enhancement in the overall performance of DSSC. The photon absorption is maximal near the electrode, with the smallest reflective value and maximum in the centre of the active layer [48].

The tunable energy bandgap interface in the solar cell allows the photovoltaic layer to produce electron-hole pairs. The ZnO&dye layer attracts the electrons, while the NiO layer attracts the holes [49]. As a consequence of this, it is important to emphasize once more that the number density of available photons passing through the layer can be affected by the following factors: (1) absorbed photons in all previous or same layers; (2) photons successfully converted into free carriers in all previous layers; and (3) reflected photons from the ITO surface.

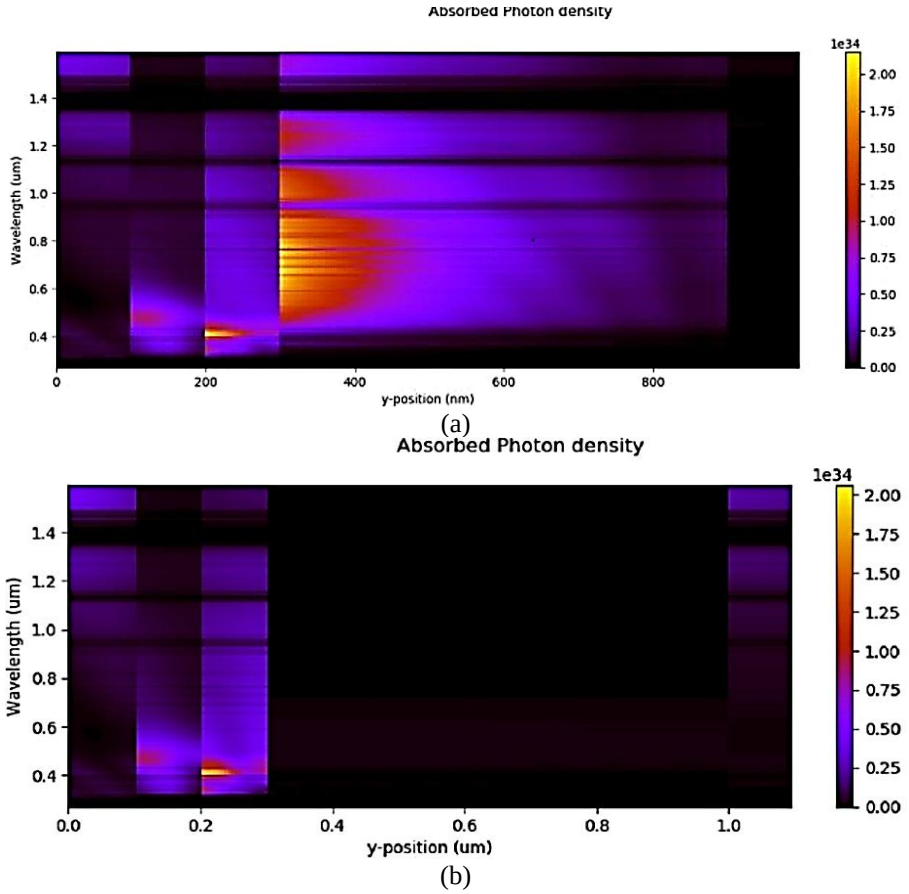


Figure 4. Absorbed photon distribution in an active region of: (a) gold-doped NiO and (b) pure NiO as an active layer at the optimized thickness of 700 and 600 nm, respectively

4. CONCLUSION

DSSCs structure of FTO/ZnO&N719/Electrolyte/NiO/FTO was simulated using OghmaNano simulation software. The effect of different types of NiO was studied with varying thicknesses from 100 nm to 1000 nm to find the highest efficiency. From the simulation results, gold-doped NiO has the best power conversion efficiency of 15.9% compared a PCE of 4.53% for pure NiO. The recombination rate of electron pairs and holes was discovered to depend on the thickness of the active layer. Therefore, gold was the best material for the counter electrode to be doped with NiO to achieve the best DSSC efficiency.

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