

# Plant-Mediated Synthesis of TiO<sub>2</sub>-ZnO Nanocomposites Using *Nigella sativa* Seeds for Solar Energy Applications

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**Abstract:** The present study introduces a novel and environmentally sustainable approach to synthesizing TiO<sub>2</sub>-ZnO nanocomposites using *Nigella sativa* seed extract, which has not been previously reported in the context of solar cell applications. This green synthesis technique uses the natural phytochemicals found in *Nigella sativa* seeds as stabilizing and reducing agents, in contrast to traditional chemical synthesis methods that frequently use hazardous chemicals and energy-intensive procedures. These bioactive compounds not only promote the formation of nanocomposites but also aid in functionalizing their surface, thereby enhancing their chemical stability and charge transfer properties. Furthermore, the incorporation of both TiO<sub>2</sub> and ZnO in a heterostructured nanocomposite is particularly advantageous, as it combines the high photoactivity of TiO<sub>2</sub> with the excellent electron mobility of ZnO. This synergistic effect leads to improved light absorption, reduced electron-hole recombination, and enhanced charge transport key factors in the performance of solar cells. The study stands out by integrating material synthesis, phytochemical surface modification, and optoelectronic property evaluation, including UV-Visible spectrographic analysis, cyclic voltammetry (CV) and current-voltage (I-V) analysis. These findings highlight the significant potential of *Nigella sativa*-mediated TiO<sub>2</sub>-ZnO nanocomposites as cost-effective, eco-friendly, and high-performance materials for next-generation photovoltaic devices.

**Keywords:** TiO<sub>2</sub>:ZnO nanocomposite, *Nigella sativa*, XRD Analysis, FTIR Analysis, UV-Visible(UV), Cyclic Voltammetry (CV), Current-Voltage (I-V), Solar Cell Performance

## 1. Introduction

Silicon wafers serve as the foundation for most solar cells on the market today, known as "first-generation" technology. The silicon wafers, which are strengthened by low-iron glass cover sheets and other system components, constitute more than half of the technology's total price. As the photovoltaic industry develops further, this cost trend is anticipated to continue [1]. The most important first step in comprehending solar energy is the transformation of solar radiation into electrical power. The photovoltaic effect, which Becquerel originally noticed in the middle of the 1950s, is what drives this process [2]. The creation of an electric voltage between two electrodes connected to a solid or liquid system in response to light exposure is the fundamental characteristic of a photovoltaic system. A pn-junction in a semiconductor is used in almost all photovoltaic devices to create and increase solar power. Solar cells are a frequent name

for these devices. The semiconductor material's capacity to absorb a sizable amount of the solar spectrum is a crucial factor. The degree to which light is absorbed close to the surface depends on the absorption characteristics. The electric field at the junction creates and separates electron-hole pairs when light is absorbed. Additionally, even for weakly absorbing materials like silicon, where the majority of carriers are generated near the surface, semiconductors should promote carrier generation as close to the surface as feasible [1]. Solar cells are typically packaged into modules, which are made up of either a thin-film material layer with series connections or several crystalline silicon cells connected in series. These modules give more voltage than a single cell. A single cell usually gives less than 1 volt. These modules also keep the solar cells safe from environmental dangers [2].

The plant *Nigella sativa* belongs to the Ranunculaceae family. People know it by many names, like Kalonji, black cumin, and seeds of blessing. Black cumin seeds grow all over the world. They are very common in the Middle East. People call this plant "miraculous" because it has a special chemical make-up. *Nigella sativa* (NS) found use in medicine for many centuries. Its use dates back to ancient times. Its therapeutic effects are largely attributed to thymoquinone (TQ), a compound with anti-inflammatory and antioxidant properties. Numerous studies have demonstrated that black cumin seeds possess protective effects against bacterial, fungal, and viral infections [3]. As one of the most important medicinal plants, black cumin has a wide range of applications. It is used either whole or crushed for various purposes. Essential oils and oleoresins are extracted using specialized techniques to produce value-added products. Additionally, black cumin seeds are traditionally used to treat ailments such as paralysis, diarrhea, jaundice, amenorrhea, helminthiasis, and asthma [4].

A common inorganic constituent in many manufacturing processes is zinc oxide. Cement, lubricants, paints, ointments, adhesives, sealants, pigments, rubbers, plastics, ceramics, glass, batteries, ferrites, fire retardants and first aid tapes are among the products that contain it. The majority of zinc oxide is made synthetically, although it does occur naturally as the mineral zincite [5-7]. Numerous studies have reported on the manufacture of ZnO nanoparticles and their potential uses in biological sciences and solar cells. Because of their high biocompatibility with human cells and toxicity to microorganisms, they are being used as antibacterial agents. Numerous chemical techniques, including chemical precipitation, sonochemical synthesis, solvothermal procedures, sol-gel processes and hydrothermal decomposition, can be used to create nanoparticles. Because of its ease of use, environmental friendliness and wide range of antibacterial activity, the biological synthesis of ZnO nanoparticles is becoming more and more significant among these [5, 8].

Recently, titanium ( $\text{TiO}_2$ ) has attracted a lot of attention because of its special qualities, such as electrical and optical ones, which are essential for a number of exciting applications, such as gas sensors and photo-electrodes. [9-11]. In general, there are three crystalline phases of  $\text{TiO}_2$ : rutile, brookite, and anatase. Only rutile and anatase are extensively utilized in a variety of technological applications [12].

## 2. Experimental details

### 2.1 Material and methods

Pyrrole, titanium isopropoxide (99.99% purity), and zinc oxide ( $\text{ZnO}$ , 99.997% purity) were the compounds utilized in this investigation. They were purchased from Sigma-Aldrich in Germany and used without any additional purification. Deionized water was used to prepare all of the solutions.

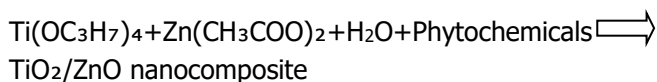
### 2.2 Preparation of *Nigella Sativa* Extract

The novelty in this preparation method lies in the use of locally sourced *Nigella sativa* seeds from Sivagiri for the green synthesis of metal oxide nanocomposites. The extract, obtained through a simple boiling process, is rich in natural phytochemicals such as flavonoids, phenolics, and alkaloids, which act as natural reducing, stabilizing, and capping agents. The dark color change observed in the emulsion suggests the successful release of these bioactive compounds, which are essential in mediating the formation of nanostructures. This approach is cost-effective, non-toxic, and environmentally friendly, making it a sustainable alternative to conventional chemical synthesis routes.

### 2.3 Preparation of $\text{TiO}_2$ : ZnO nanocomposite with seeds extract

A magnetic stirrer was used to dissolve 5 g of zinc acetate in 100 mL of distilled water and agitate the mixture for 30 minutes in order to create pure ZnO nanoparticles. Separately, 100 mL of distilled water was mixed with 5 mL of titanium isopropoxide, and the mixture was swirled for half an hour. The prepared zinc solution was then slowly added to the titanium solution under continuous stirring for another 30 minutes. 3 g of NaOH was added dropwise to bring the mixture's pH down to 10. A white aqueous  $\text{TiO}_2$ -ZnO solution was formed after the solution was agitated for another half hour to maintain the optimum pH. Then, 20 mL of *Nigella sativa* seed extract was added into the titanium and zinc precursor solution. This solution was mixed for thirty minutes. After adding the plant extract, the solution slowly turned bright black. The mixture kept undisturbed at room temperature for a full day. The settled material was dried. This drying took three hours at  $70^\circ\text{C}$ , using a hot air oven. Finally, a light black powder formed. This powder was the  $\text{TiO}_2$ -ZnO nanocomposite.

## 2.3 Chemical Reaction



## 2.4 Characterization Techniques

A Shimadzu FTIR Prestige-21 spectrophotometer measured the FTIR spectra of the created compounds. Similarly, a Shimadzu UV-1800 spectrophotometer measured the UV-visible absorption spectra of these materials [13]. For the nanocomposites, a Scintag XDS-2000 diffractometer helped obtain the X-ray diffraction (XRD) patterns [14].

## 3. Result and Discussion

### 3.1 XRD Analysis

Figure 1 shows the XRD pattern for the TiO<sub>2</sub>/ZnO nanocomposite material. For easy comparison, this figure also has reference patterns. These include wurtzite-phase ZnO (JCPDS card no. 36-1451) and brookite-phase TiO<sub>2</sub> (orthorhombic, JCPDS card no. 29-1360). The crystallite size of the nanoparticles was found. This calculation used the main diffraction peak and the Debye–Scherrer equation. Distinct diffraction peaks of the TiO<sub>2</sub>/ZnO (TZN) nanocomposite were observed at 2θ values of 36.42°, 37.86°, 40.74°, 54.89°, 70.96°, 31.14°,

36.50°, 47.65°, 56.37°, 66.69°, 69.52°, and 72.96°. These peaks correspond to the (012), (131), (022), (320), (332), (100), (101), (102), (110), (200), (201), and (004) crystallographic planes, respectively [15]. The XRD pattern confirms that the nanocomposite system formed correctly. It shows characteristic peaks for both TiO<sub>2</sub> and ZnO phases. The strongest diffraction peaks belong to the brookite phase of TiO<sub>2</sub>. Other peaks, for example, the one at 37.86°, point to the presence of both hexagonal (ZnO) and orthorhombic (TiO<sub>2</sub>) phases inside the composite. Previous research describes this observation [16]. The crystallite size was found from the XRD pattern. Scherer's formula helped in this determination.

$$D = K\lambda / \beta \cos \theta \text{ (nm)}$$

### 3.2 Fourier-Transform Infrared Spectroscopy (Ftir)

The FTIR spectra of TiO<sub>2</sub>-ZnO (TZN) nanocomposites are reported in Table 1 and Figure 2. The wavenumber range in which the spectra were recorded was 4000 cm<sup>-1</sup> to 500 cm<sup>-1</sup>. The spectrum's absorption peaks show that different functional groups are present. A noticeable broad band at 3454 cm<sup>-1</sup> that corresponds to O–H stretching vibrations indicates the presence of hydroxyl groups, possibly from absorbed water or plant phytochemicals.

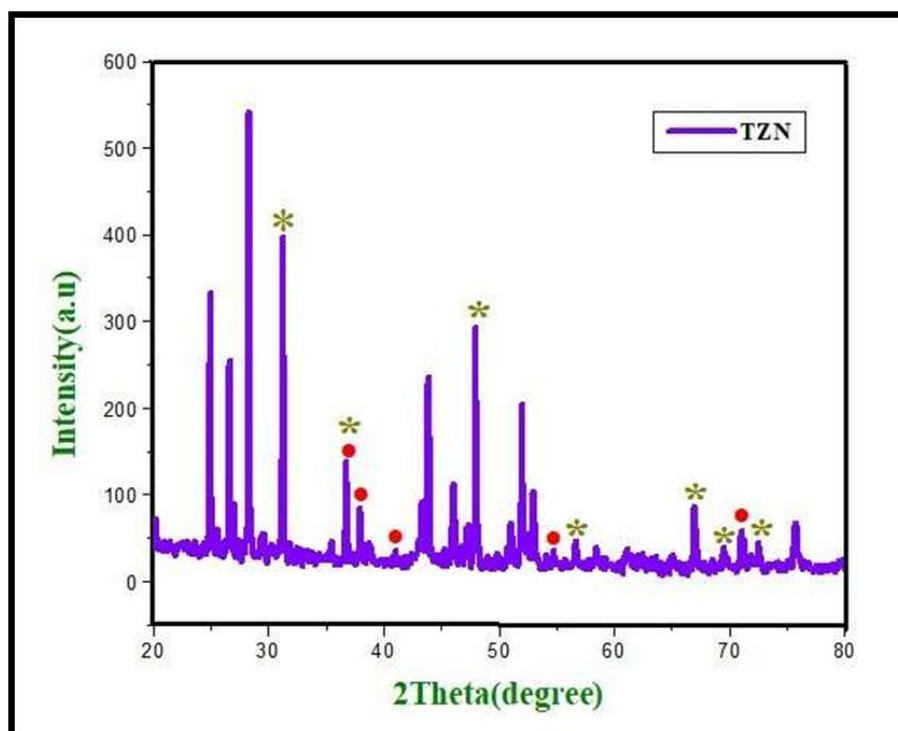
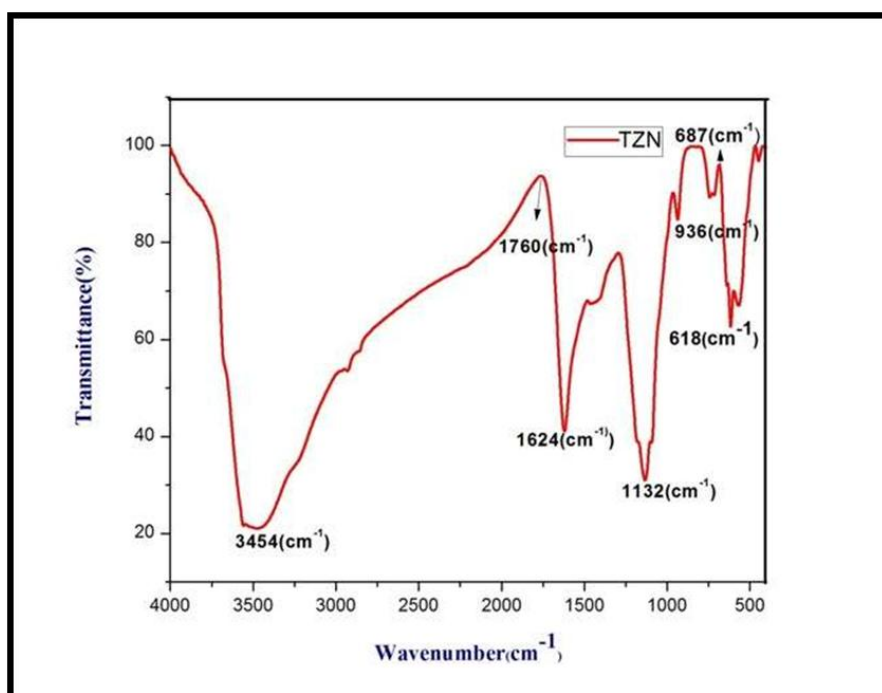


Figure 1. XRD analysis of TZN Nanoparticles

**Table 1.** FTIR Spectrum of TZN Nanoparticles

S.No	Bond range( $\text{cm}^{-1}$ )	Type of vibration	Inferences
1	3454( $\text{cm}^{-1}$ )	OH Sterching(bonded)	Observed when steric Hinderance prevents polymeric association
2	1760( $\text{cm}^{-1}$ )	-do-	4-Ring Saturated
3	1624( $\text{cm}^{-1}$ )	N-O Streching	Higher one assigned to trans and lower to cis
4	1132( $\text{cm}^{-1}$ )	SO <sub>2</sub> Symmetric Stretching	Sulphones
5	936( $\text{cm}^{-1}$ )	N-O Stretching	In quinine monoximes shifted to 1075-925 $\text{cm}^{-1}$ because of contribution of C=N-OH
6	687( $\text{cm}^{-1}$ )	O-H=O bending	For cis form
7	618( $\text{cm}^{-1}$ )	OCN deformation	Amide Present

**Figure 2.** FTIR Spectrum of TiO<sub>2</sub>:ZnO Nanocomposite

The symmetric C=O stretching is responsible for the band at 1760  $\text{cm}^{-1}$ . Other significant peaks include a band at 1624  $\text{cm}^{-1}$ , corresponding to C=C stretching, a band at 1132  $\text{cm}^{-1}$  indicating symmetric stretching of SO<sub>2</sub> groups, and a peak at 936  $\text{cm}^{-1}$  assigned to N-O stretching. The peak at 687  $\text{cm}^{-1}$  is related to O-H=O bending vibrations. Notably, the band observed at 618  $\text{cm}^{-1}$  may be associated with OCN deformation or could also correspond to the stretching vibrations of Ti-Zn-O bonds in the synthesized nanocomposite. These spectral characteristics confirm the successful preparation of TZN nanocomposite and provide valuable information

concerning molecular interactions and surface functional groups dominating the material. The KBr technique was used to make FTIR measurements in the wave number range of 4000-500  $\text{cm}^{-1}$  in reported work [17].

### 3.3 Uv-Visible Spectrophotometer Analysis

The absorption band is shifted into the visible range in the optical absorption spectra of TiO<sub>2</sub>-ZnO nanocomposites, as evident in Figure 3. The agglomeration in the suspension results in the change in absorption intensity, and sediment formation during



synthesis resulted in the decrease in absorbance. This is prominently seen in TiO<sub>2</sub>-ZnO nanoparticles synthesized from *Nigella sativa* seed extract. A wavelength of maximum absorption around 234 nm was observed, which is attributed to electronic transitions between localized states within the energy band gap. The energy states can be attributed to structural defects incorporated during the synthesis of the nanocomposite. Such types of defects dictate the band gap of TiO<sub>2</sub>-ZnO nanocomposites synthesized from *Nigella sativa*. In addition, red shift in the absorption edge occurs with an increase in the volume ratio of TiO<sub>2</sub> to ZnO, suggesting better absorption of visible light. The band of absorption at 234 nm is related to electronic transitions caused by deep levels of the valence band. In addition, earlier research has also indicated that *Nigella sativa* has a strong absorbance within the 200–800 nm range, which could improve the light-harvesting capability of the nanocomposite [18].

### 3.4. Cyclic Voltammetry (C-V)

The electrochemical activity of TiO<sub>2</sub>-ZnO nanocomposites prepared from *Nigella sativa* seed extract may be characterized more effectively by the technique of Cyclic Voltammetry (CV) measurement, as needed for solar cell applications (Figure 4). Active

electron transfer mechanisms within the nanocomposite are indicated by the different redox peaks on the CV plot with current (I) as the parameter plotted against potential (V). The effective charge storage and transfer capability of the TiO<sub>2</sub>-ZnO system is indicated by the presence of defined anodic and cathodic peaks. With the addition of *Nigella sativa* seed extract, rich in bioactive phytochemicals, structural stability and electrical conductivity of material are enhanced and thus improve the charge transfer kinetics. The enhanced high electrochemical activity of nanocomposite is confirmed with higher peak current density and wider peak separation in comparison to pure ZnO or TiO<sub>2</sub>. As greater charge separation and lesser electron-hole recombination assisted greater power conversion efficiency in solar cell devices, this amplified redox activity is directly correlated with amplified photovoltaic functionality [13].

### 3.5. Current Voltage (I-V)

The I-V characteristics of the TiO<sub>2</sub>-ZnO nanocomposites containing *Nigella sativa* seed extract were investigated in the presence of sunlight. The current-voltage (I-V) curve showed an enhanced photocurrent response, indicating higher charge carrier separation and transport efficiency.

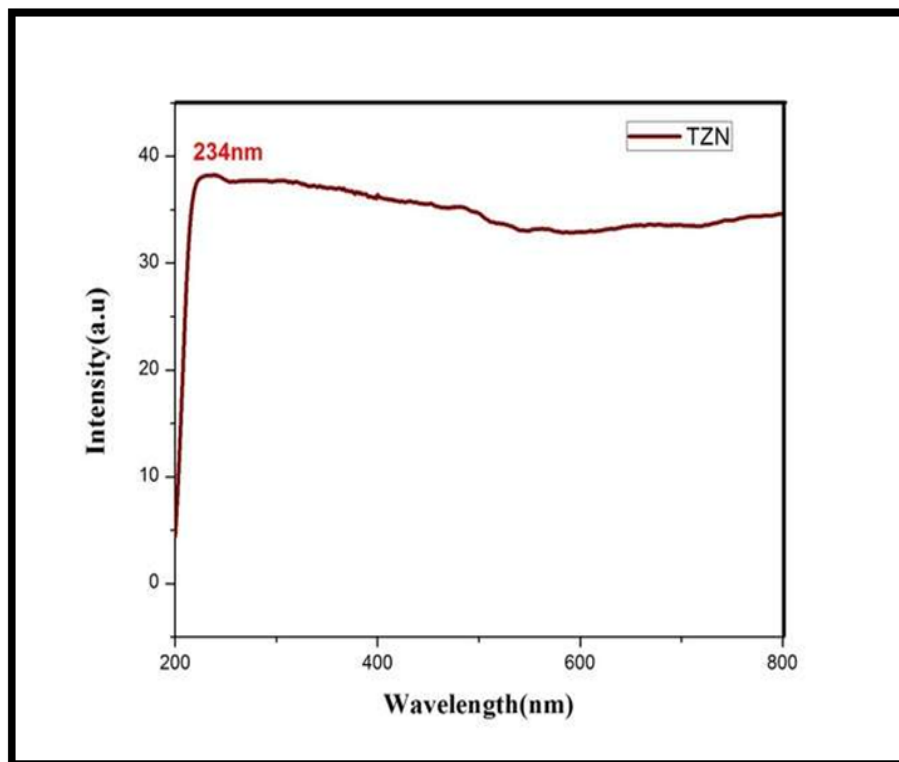
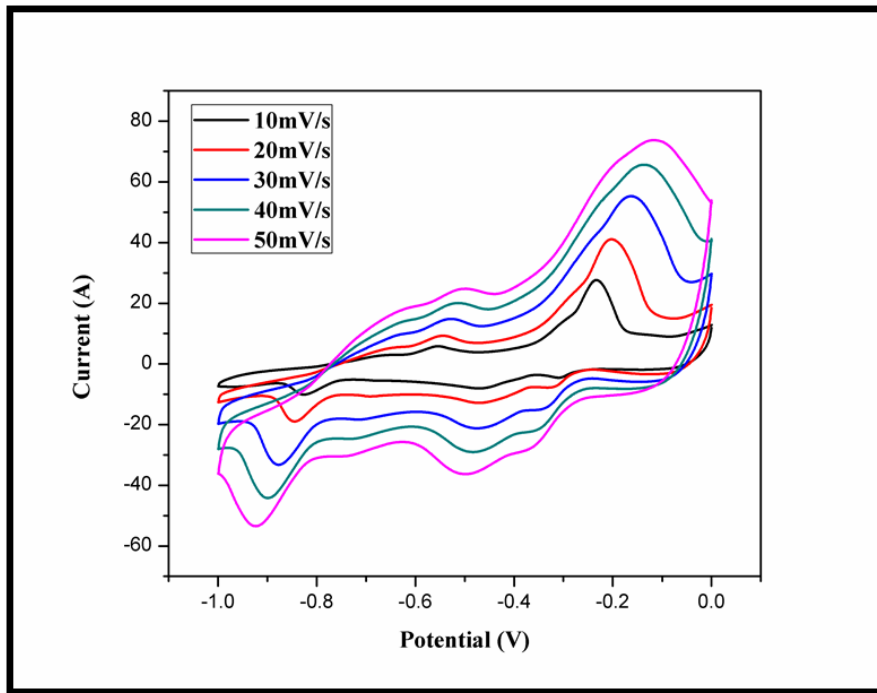
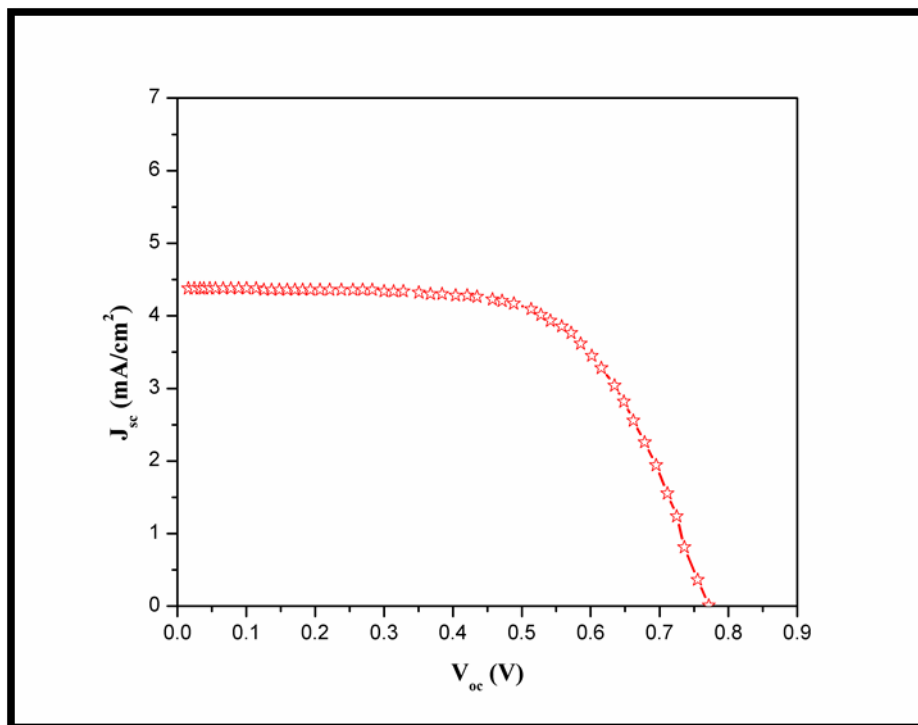


Figure 3. UV-Visible spectrum wavelength



**Figure 4.** Cyclic Voltammetry (CV)



**Figure 5.** Current Voltage (I-V)

**Table 2.** I-V Characteristics of TiO<sub>2</sub>:ZnO Nanocomposites Solar Cell

Sample	V <sub>oc</sub> (V)	J <sub>sc</sub> (mA/cm <sup>2</sup> )	Fill factor (ff)	Efficiency (%)
TZN	0.76	4.31	0.60	2.42

The nanocomposite's heterojunction structure shows a clear improvement in both open-circuit voltage (V<sub>oc</sub>) and short-circuit current density (J<sub>sc</sub>). This happens due to a combined effect. This effect is not

seen in pure TiO<sub>2</sub> or ZnO alone. Also, the Nigella sativa extract has phytochemicals. These phytochemicals work as organic stabilizers and reducers. They improve interface properties. They also reduce electron-hole



recombination losses. These outcomes show that the TiO<sub>2</sub>-ZnO nanocomposite is a good material (Figure 5). It suits solar cell uses where high efficiency is important.

The I-V properties of the TiO<sub>2</sub>-ZnO nanocomposites were studied (Table 2). These nanocomposites were made with *Nigella sativa* seed extract. The study happened under simulated solar light. Photovoltaic performance was judged using current-voltage measurements. This included power conversion efficiency (PCE), fill factor (FF), open-circuit voltage (V<sub>oc</sub>) and short-circuit current density (J<sub>sc</sub>).

#### 4. Conclusion

Green reducing and stabilizing agent *Nigella sativa* seed extract helped to synthesis TiO<sub>2</sub>-ZnO nanocomposites successfully. X-ray diffraction (XRD) studies confirmed the nanocomposite's crystal structure. These crystals were small, which gave a large surface area. Fourier-transform infrared (FTIR) spectroscopy found functional groups from the extract. This showed that the nanoparticles were stable. UV-visible spectroscopy proved better light absorption. This makes the material good for solar cell applications. Cyclic voltammetry (CV) showed improved electrochemical activity. Current-voltage (I-V) characteristics displayed better charge transport. The nanocomposites had higher electron movement and less recombination. This led to their excellent solar efficiency. This method uses an eco-friendly synthesis. It is a cost-effective way for renewable energy usage. This path offers a sustainable technology. Therefore, these bio-assisted TiO<sub>2</sub>-ZnO nanocomposites hold great promise for future solar cell technologies.

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#### Conflict of interest

The Authors declares that there is no conflict of interest anywhere.

#### Does this article screened for similarity?

Yes

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#### Author Contribution Statement

S. Srimathi: Conceptualization, Methodology, Validation, Formal Analysis, Investigation. V. Kalaiselvi: Formal Analysis, Investigation, Writing-Original Draft,