



Temperature-induced Modifications in Tungsten Oxide Nanoparticles and their Effect on the Efficiency of Dye-sensitized Solar Cells

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ABSTRACT

This study investigates the synthesis and characterization of tungsten oxide (WO₃) nanoparticles, with a particular focus on the influence of varying annealing temperatures (100°C, 150°C, and 200°C) on their properties and performance in dye-sensitized solar cells (DSSCs). The WO₃ nanoparticles were synthesized using a simple chemical method and characterized through X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV-Vis spectroscopy, and Fourier-transform infrared spectroscopy (FTIR). The results indicated that higher annealing temperatures led to an increase in crystalline size and improved crystallinity. The band gap energies were found to increase slightly with higher temperatures, influencing the optical absorption properties. XRD analyses revealed temperature-dependent morphological changes, with particle sizes ranging from 38.1 nm to 46.9 nm. The photovoltaic performance of DSSCs incorporating WO₃ nanoparticles demonstrated enhanced efficiency with increasing annealing temperature, achieving a maximum efficiency of 0.0093% at 200°C. These findings provide valuable insights into optimizing WO₃ nanoparticles for diverse applications, particularly in energy conversion technologies.

Keywords: Tungsten oxide nanoparticles; Dye-sensitized solar cells; Annealing temperature; Photovoltaic efficiency; Morphological characteristics.

1. INTRODUCTION

Nanomaterials have become integral in various technological advancements, particularly in energy storage systems, threat detection in defence and navy applications, drug delivery mechanisms, and water purification processes. Among these materials, transition metal oxides like tungsten oxide (WO₃), titanium oxide (TiO₂), and zinc oxide (ZnO) stand out for their functional properties and versatile applications, especially when engineered into nanoparticles. WO₃, in particular, is renowned as an n-type semiconducting material, making it a focal point for nanoparticle synthesis due to its eco-friendliness and robust chemical stability. Its cost-effectiveness and moderate band gap energy of approximately 3 eV has spurred extensive research, leading to a broad spectrum of applications spanning from dye-sensitized solar cells to medical devices, electrochromic systems, photochromic materials, thermochromic applications, gasochromic sensors, and photocatalysts for water splitting and gas sensing (Santos *et al.* 2016; Tsuyumoto *et al.* 2018).

Recent studies underscore the significance of WO₃ nanoparticles in electrochemical and optoelectronic

applications, particularly due to their high charge carrier mobility. This characteristic makes WO₃ a valuable material for electrochemical devices and as a photoelectrode in dye-sensitized solar cells (DSSC) (Babu *et al.* 2021; Huang *et al.* 2021; Yong *et al.* 2013). The band gap of WO₃, which aligns well within the solar spectrum, enhances its photocatalytic activity for solar-driven applications, such as solar photoconductivity and water splitting. These properties have demonstrated promising results in solar energy harvesting technologies, marking WO₃ as a highly effective candidate for DSSCs and other applications in renewable energy (Fang-Bai *et al.* 2000; Rout *et al.* 2006; Wang *et al.* 2023; Zhang *et al.* 2023).

In recent years, significant efforts have focused on refining synthesis methods for WO₃ nanoparticles to achieve improved control over particle size, morphology, and surface characteristics, optimising their performance in DSSCs and other applications. A variety of techniques have been explored, including gas condensation, vacuum deposition, vaporization techniques, chemical vapour deposition (CVD), chemical vapour condensation (CVC), sol-gel processing, hydrothermal synthesis, mechanical attrition, and electro-deposition (Andrievskii

et al. 1994; Desseigne *et al.* 2019; Dikumar *et al.* 2009; Hasany *et al.* 2013; Gohil *et al.* 2007; Konrad *et al.* 2001; Saini *et al.* 2024; Shabdan *et al.* 2024). Among these, simple chemical methods remain highly popular due to their simplicity, low cost, scalability, and rapidity, producing WO₃ nanoparticles with high purity and the desired properties. These methods are particularly advantageous for large-scale production, making them a practical choice for developing WO₃ nanoparticles tailored for advanced technological applications.

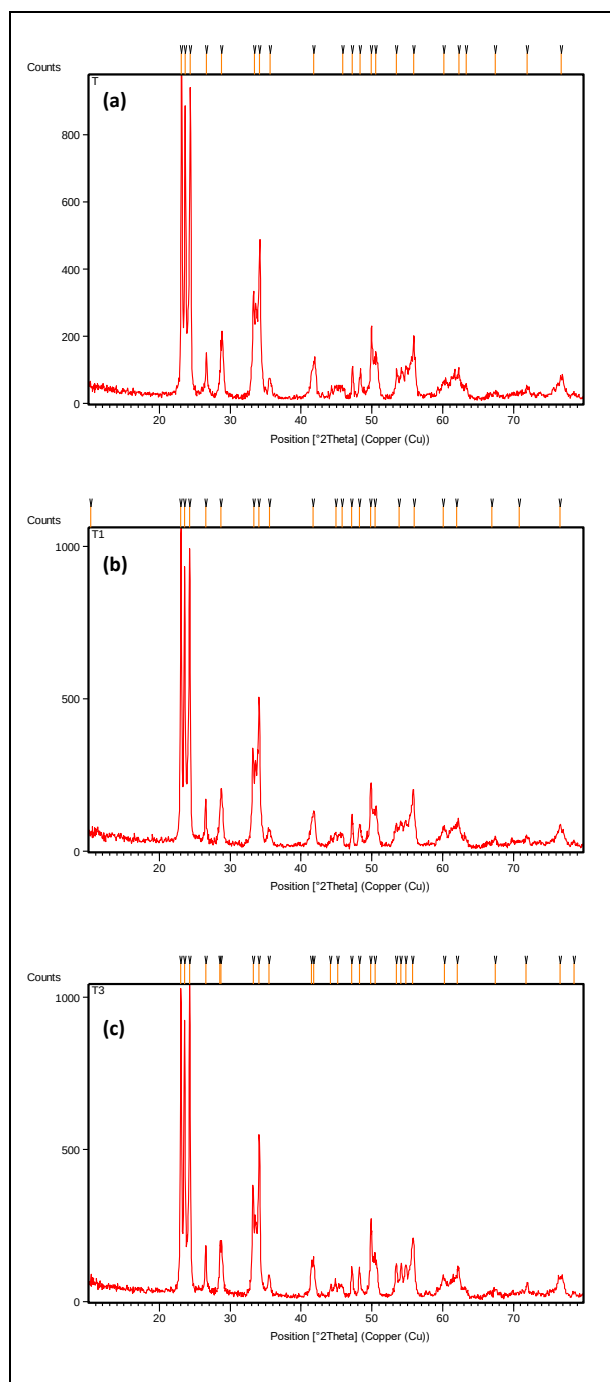


Fig. 1: XRD patterns of WO₃ nanoparticles annealed at (a) 100 °C, (b) 150 °C and (c) 200 °C

This study seeks to address a gap in current research by investigating the effects of temperature on the structural and functional properties of WO₃ nanoparticles. By examining their thermal characteristics, the research aims to provide insights into how varying temperature conditions influence WO₃ nanoparticle properties, with implications for optimising their performance in energy storage, electrochromic devices, and DSSCs. This work builds on recent advancements and contributes foundational knowledge on WO₃ nanoparticles' behaviour under different thermal conditions, paving the way for their enhanced utilisation and tailored design in future technological applications.

2. EXPERIMENTAL

2.1 Chemicals and Instruments

All reagents used were of analytical reagent grade without further purification. Tungsten chloride (99.99%) and cyclohexanol were obtained from Sigma Aldrich suppliers in India.

X-ray diffraction studies were conducted using a PANalytical X-ray diffractometer with nickel-filtered CuK α radiation (30 kV, 30 mA). The surface morphology of the samples was examined using scanning electron microscopy (SEM; S-4100, Hitachi). The optical properties were investigated using absorbance spectra recorded by a Cary 500 spectrometer. The FTIR spectrum was recorded using the palletisation method in the range 400–4,000 cm⁻¹ with a Shimadzu FTIR spectrometer. The functional groups present in the WO₃ nanoparticles were confirmed by Raman Spectroscopy (RA400, Mettler Toledo). The current–voltage (I–V) characteristics were measured using white light from a xenon lamp (maximum 150 W) with a Sun 2000 solar simulator (ABE Technologies). Light intensity was adjusted using a Si solar cell to approximately AM-1.5. Incident light intensity and active cell area were 100 mW cm⁻² (one sun illumination) and 0.25 cm² (0.5 x 0.5 cm), respectively.

2.2 Synthesis of WO₃ Nanoparticles

A quantity of 25 mg of tungsten chloride was dissolved slowly in 5 ml of cyclohexanol with continuous stirring using a magnetic stirrer until a uniform solution was achieved. Initially, the solution exhibited a yellow color, which gradually turned white after 45 minutes of stirring. Subsequently, the white color transformed into a sky blue hue within 60 minutes of continuous stirring. The stirring process was continued until the solution darkened to a deep blue color, indicating the formation of WO₃ nanoparticles. The resulting solution was centrifuged and washed with distilled water to attain a neutral pH. Following this step, the nanoparticles settled at the bottom of the centrifugal tube and were subjected to slow evaporation at room temperature to remove

excess solvent. Finally, the WO₃ nanoparticles were collected and placed in a 125 ml Teflon-lined stainless steel autoclave, where they were exposed to temperatures of 100°C, 150°C, and 200°C for a duration of 5 hours.

2.3 Sample Preparation for Solar Cell

The preparation of the WO₃-based paste for DSSCs involved using WO₃ nanoparticles synthesized at varying temperatures (100°C, 150°C, and 200°C). To prepare the paste, 0.5 grams of WO₃ powder was combined with a solution containing 6 grams of α -terpineol, 1 gram of cellulose, and 25 ml of ethanol. This mixture underwent sonication for 18 hours at intensity of 1,500 Wcm⁻² to ensure uniform dispersion.

2.4 Device Fabrication Procedure

The fluorine-doped tin oxide (FTO) conducting glass substrates (Hartford FTO, $\sim 30\Omega\text{ cm}^{-2}$ resistance, 80% transmittance in the visible range) were thoroughly cleaned by sequential rinsing with acetone, ethanol, and deionized water, followed by 15 minutes of ultrasonic treatment in each solvent to remove surface contaminants. The WO₃ paste, prepared previously, was applied onto the cleaned FTO substrates using the doctor blade technique to achieve a uniform film, air-dried, and then annealed at 350°C for 30 minutes to enhance adhesion and crystallinity. The annealed WO₃-coated substrates were immersed in an N719 dye solution in ethanol for 24 hours in the dark to ensure effective dye loading. For the counter electrode, a platinum layer was deposited on an FTO glass by drop-casting a solution of H₂PtCl₆, followed by thermal annealing at 400°C for 15 minutes. Finally, the dyed sensitized WO₃-coated photoelectrode and platinum counter electrode were assembled into a sandwich-type structure with a thin polymer spacer, and an iodide/triiodide electrolyte solution was injected to complete the DSSC assembly.

3. RESULTS AND DISCUSSIONS

3.1 XRD Analysis

XRD pattern of the synthesized WO₃ nanoparticles at different temperatures are shown in Figure. 1. The X-ray diffraction analysis of the WO₃ sample annealed at 100°C revealed distinct crystalline peaks at 23.04°, 23.54°, and 24.24°, which were successfully indexed and matched with the JCPDS (05-0363) data. Minor variations in the 2 θ values were observed due to the annealing process. According to Debye Scherrer's formula, the average crystallite size for the 100°C annealed sample was determined to be 38.1 nm. As the annealing temperature increased to 150°C and 200°C, there was a noticeable increase in the crystallite size, measured at 43.3 nm and

46.9 nm, respectively. Additionally, the intensity of the prominent peaks also increased with higher annealing temperatures, indicating improved crystallinity correlated with larger particle sizes. These findings illustrate the direct relationship between crystallinity and particle size, demonstrating that increasing annealing temperatures leads to enhanced crystalline properties and larger particle sizes. Table 1 summarizes the 2 θ values, corresponding d-spacings, relative intensities, and average particle sizes of the WO₃ nanoparticles at different annealing temperatures.

Table 1. 2 θ values, corresponding d-spacings, relative intensities, and average particle sizes of the WO₃ nanoparticles at different annealing temperatures

Temperature (°C)	2 θ (degree)	d - spacing (Å)	Relative intensity (%)	D (nm)	Average particle size (nm)
100	23.041	3.85	100	38.0	38.1
	23.547	3.77	96.3	42.6	
	24.247	3.66	96.44	37.5	
150	23.03	3.85	93.15	41.2	43.3
	23.533	3.77	87.6	40.9	
	24.262	3.66	100	47.7	
200	22.982	3.86	100	42.5	46.9
	23.492	3.78	91.94	47.6	
	24.22	3.67	93.71	50.6	

3.2 Morphological Analysis of WO₃ Nanoparticles

The surface morphology of WO₃ nanoparticles is depicted in the SEM images shown in Figures 2b-d. These images reveal that the WO₃ nanoparticles have a spherical shape. The nanoparticles exhibit rough surfaces, as indicated in the images. Additionally, it is observed that the particle size increases with the rising annealing temperature, which is consistent with the particle size values obtained from XRD analysis, as presented in Table 1. The images display a relatively homogeneous nanostructure, with both smaller and larger particles present in certain areas. This observation further supports the correlation between particle size and temperature.

Energy dispersive X-ray analysis (EDAX) pattern of the WO₃ nanoparticles prepared at 100°C is shown in Figure 2a. The EDAX spectrum shows the representative peaks of oxygen and tungsten with carbon peak from the Formvar carbon-coated grid. Figures 3a-c shows the transmission electron microscope (TEM) images of WO₃ nanoparticles annealed at different temperatures like 100°C, 150°C and 200°C, respectively. The images confirm an increase in particle size with rising temperature, consistent with the XRD and SEM results.

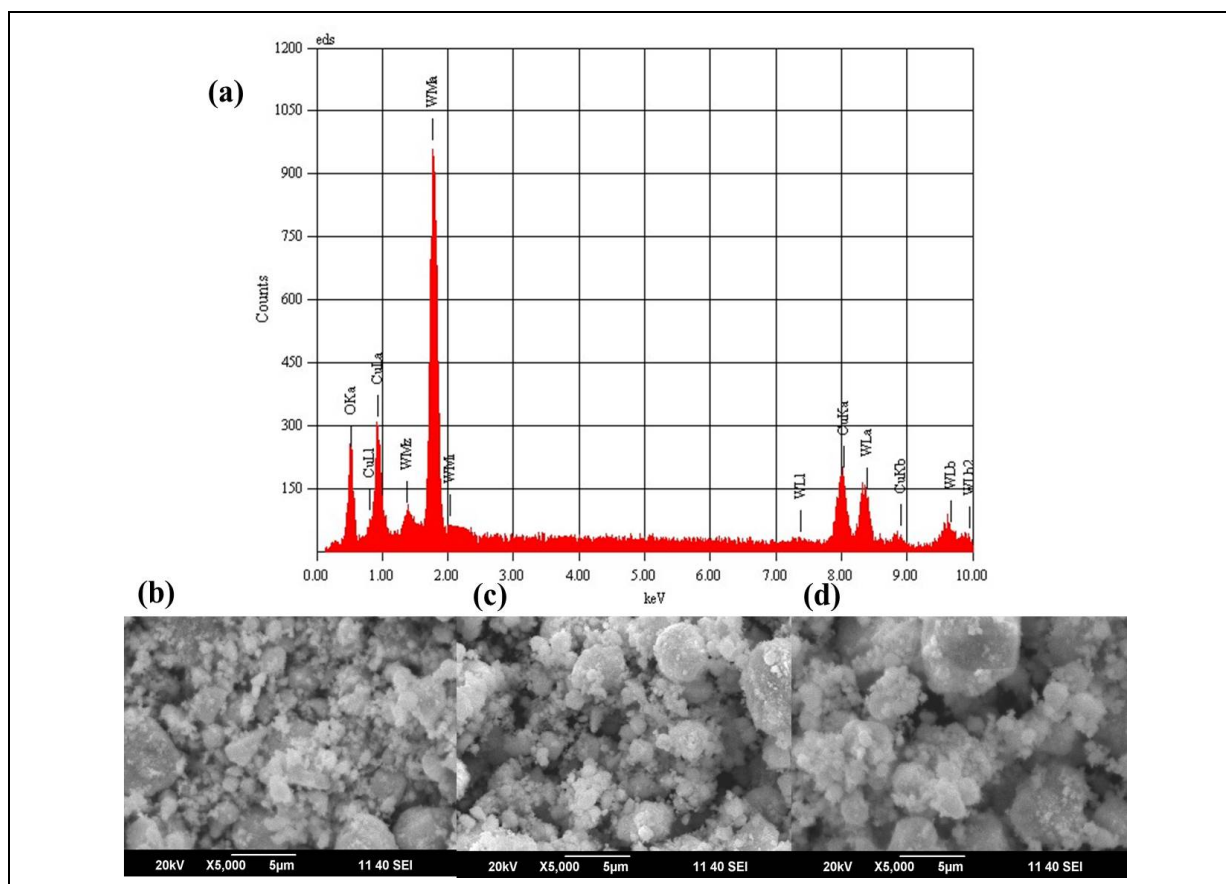


Fig. 2: (a) EDAX Spectrum of WO_3 nanoparticles annealed at 100°C; SEM images of WO_3 nanoparticles annealed at (b) 100°C, (c) 150°C and (d) 200°C temperatures.

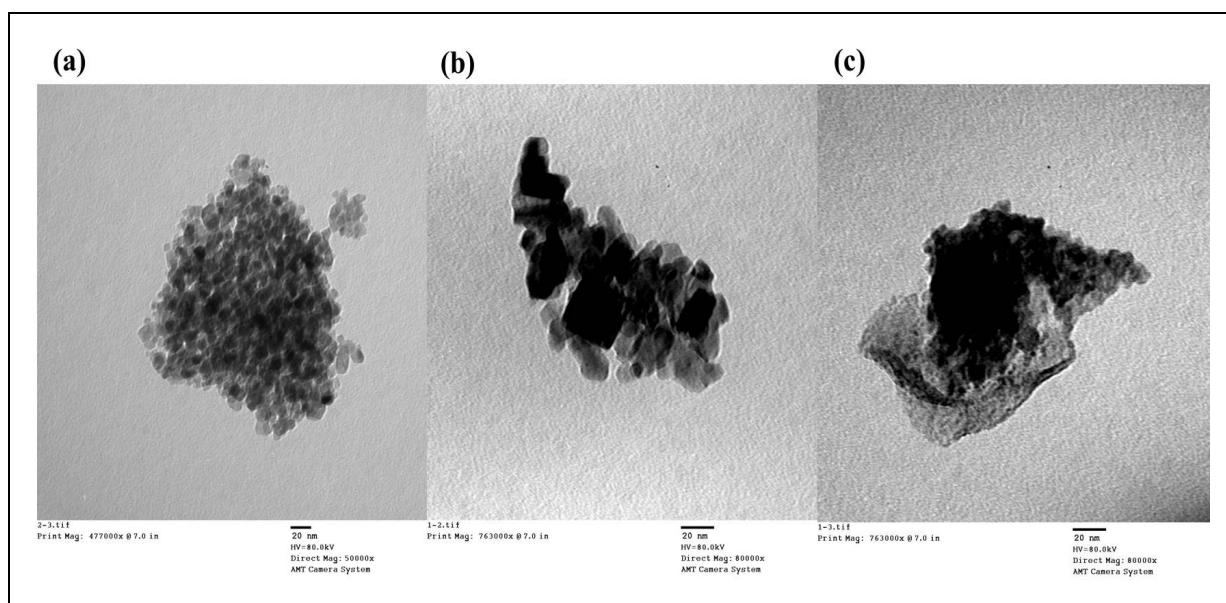


Fig. 3: TEM image of WO_3 nanoparticles annealed at (a) 100 °C, (b) 150 °C and (c) 200 °C temperatures (Scale bar 20 nm for all images)

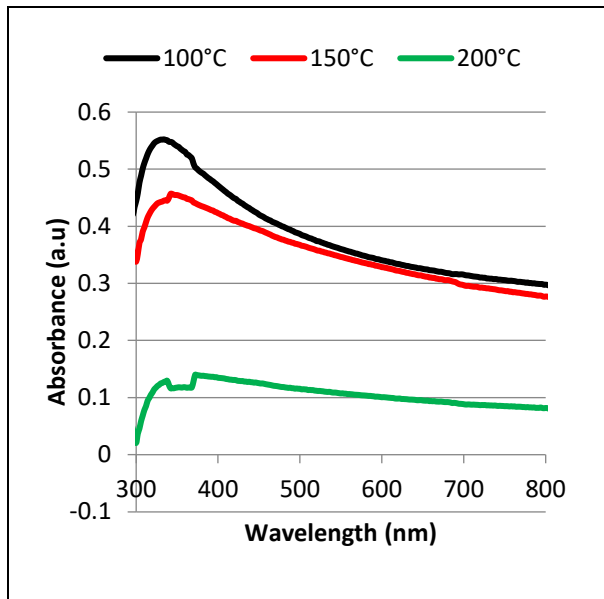


Fig. 4: UV-Vis spectral analysis of WO₃ nanoparticles annealed at different temperatures

Table 2. Variation in crystallite size and energy band gap with increasing temperature.

Temperature (°C)	Band gap (eV)
100	2.76
150	2.81
200	2.85

3.3 UV-Vis NIR Spectral Analysis of WO₃ Nanoparticles

The optical absorption properties of the WO₃ nanoparticles are analyzed from UV-visible spectroscopy and the results are presented in Figure 4. The optical properties of WO₃ nanoparticles within the visible region are governed by their transmission characteristics, which are distinctly influenced by the band gap energy of the material. Despite slight variations in particle size due to annealing temperatures, as observed in the XRD study of annealed particles, the onset position of light absorption remains relatively consistent across all particles. However, this minor change in crystallite size manifests in the UV-visible spectral data, particularly in the wavelength range of 376–398 nm, resulting in a red shift of the absorption wavelength. The band gap energy (E) is calculated using the formula $E = h\nu$ (eV), where h represents Planck's constant and ν denotes the frequency of radiation of a photon. For the 100 °C WO₃ nanoparticles, the band gap energy is approximately 2.76 eV. Similarly, the band gap energy values for the 150 °C and 200 °C WO₃ nanoparticles are measured at 2.81 eV and 2.85 eV, respectively, indicating an increase with higher annealing temperatures. This rise in band gap energy is likely attributed to the elevated temperature during annealing. The optical absorption coefficient, correlated with the calculated energy band gap of 2.76

eV, aligns well with findings from previous research (Prabhu *et al.* 2014).

3.4 FT-IR Analysis of WO₃ Nanoparticles

Fourier Transform Infrared (FT-IR) analysis stands out as a promising method for studying molecular vibrations. Figure 5 presents the FT-IR spectra of WO₃ nanoparticles synthesized at 100°C, 150°C and 200°C. FT-IR spectra offer valuable insights into both in-plane and out-of-plane segmental vibrations of atoms and molecules, correlating with their energies within the infrared (IR) region. In WO₆, tungsten (W) atoms occupy the central positions within the octahedron, while oxygen (O) atoms reside at the vertices, forming a W–O–W configuration (Pfeifer *et al.* 1995). In our investigation, we have observed fundamental vibrations corresponding to W=O, W–O and W–O–W bonds in the FT-IR spectra of WO₃ nanoparticles.

Table 3. Different functional groups and their wavenumbers in WO₃ nanoparticles

Group	Wave numbers (cm ⁻¹)	Assignments
W=O, W-O-W	400 - 500	Bending and stretching vibrations
W-O-W	845	W ₃ O ₉
W-O, W=O	900-1000	Stretching vibrations

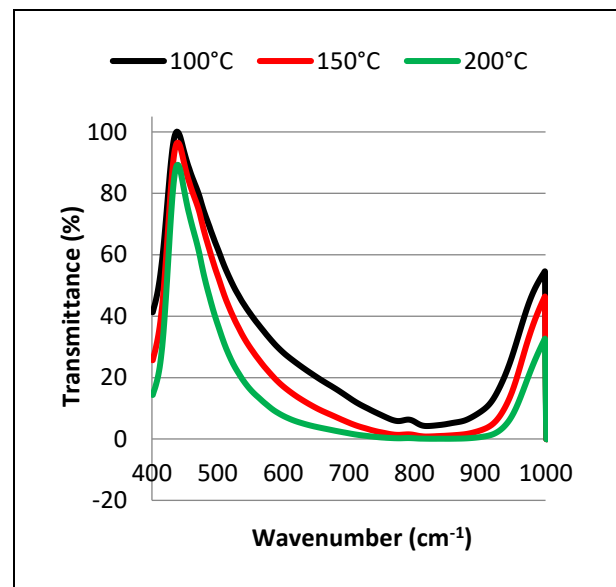


Fig. 5: FT-IR analysis of WO₃ nanoparticles annealed at different temperatures.

The FT-IR peaks observed in the range between 400 cm⁻¹ and 500 cm⁻¹ are typically associated with the metallic tungsten-oxygen stretching vibrations in WO₃ nanostructures. These vibrations arise from the stretching of W=O bonds in tungsten oxide and/or the bending or stretching of W-O-W bonds. The band observed at 845

cm^{-1} suggests the presence of W_3O_9 , which contains W-O-W bonding. Additionally, the IR absorbance peaks between 900 cm^{-1} and 1000 cm^{-1} are attributed to the W-O and W=O stretching vibrations in WO_3 nanostructures (Kumar *et al.* 2011).

3.5 I-V Characteristics of WO_3 Nanoparticles

Figure 6 displays the I-V characteristics of WO_3 nanoparticles prepared at different temperatures (100°C , 150°C and 200°C) for dye-sensitized solar cells. The solar cells utilizing WO_3 nanoparticles annealed at 100°C as a working electrode exhibit a power conversion efficiency (η) of 0.0025% with a short-circuit current density (J_{sc}) of 0.0025 mAcm^{-2} , open circuit voltage (V_{oc}) of 1.0 V, and fill factor (FF) of 1.0. Comparatively, solar cells utilizing WO_3 nanoparticles annealed at 150°C demonstrate an increased efficiency (η) of 0.0046% with J_{sc} of 0.0051 mAcm^{-2} , V_{oc} of 0.9 V, and FF of 1.0. Solar cells employing WO_3 nanoparticles annealed at 200°C exhibit further enhancement in efficiency (η) to 0.0093% with J_{sc} of 0.0125 mAcm^{-2} , V_{oc} of 0.75 V, and FF of 1.0.

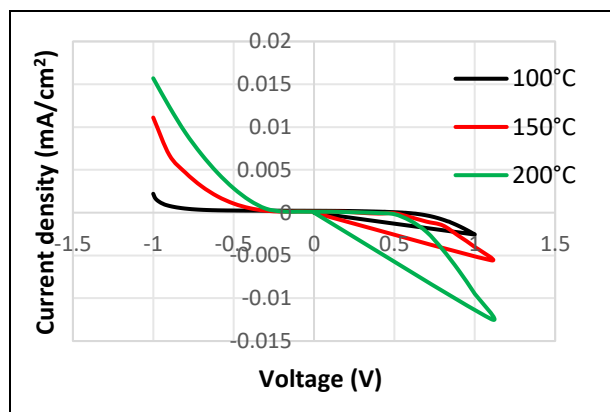


Fig. 6: I-V characteristics of WO_3 nanoparticles at different temperatures (T1- 100°C , T2- 150°C & T3- 200°C)

Table 4. Photovoltaic characteristics of the DSSCs prepared using WO_3 nanoparticles

WO_3 synthesized temperature ($^\circ\text{C}$)	J_{sc} (mAcm^{-2})	V_{oc} (V)	FF	Efficiency, η (%)
100	0.0025	1.0	1.0	0.0025
150	0.0051	0.9	1.0	0.0046
200	0.0125	0.75	1.0	0.0093

The power conversion efficiency and short-circuit current density of the solar cells show an upward trend with increasing temperature, possibly attributed to structural changes and increased particle size as evidenced in XRD, SEM and TEM images (Fig. 1, 2 and 3). The sample surface area of WO_3 nanoparticles facilitates dye adsorption, contributing to the generation of electron-hole pairs and subsequently higher short-circuit current densities. This underscores the

significance of dye adsorption by the film in influencing solar cell performance.

4. CONCLUSION

This study presents the synthesis and characterization of WO_3 nanoparticles, with a focus on the effects of annealing temperatures (100°C , 150°C , and 200°C) on their structural, optical, and photovoltaic properties. XRD analysis showed an increase in crystallite size and crystallinity with higher annealing temperatures, with average particle sizes ranging from 38.1 nm to 46.9 nm. Morphological analysis via SEM and TEM confirmed temperature-dependent changes in nanoparticle size and structure. UV-Vis spectroscopy revealed a slight increase in band gap energies from 2.76 eV to 2.85 eV with higher temperatures. FT-IR analysis indicated the presence of functional groups associated with WO_3 , and I-V characteristics demonstrated enhanced photovoltaic performance in dye-sensitized solar cells, achieving a maximum efficiency of 0.0093% at 200°C . These findings highlight the potential of WO_3 nanoparticles for improving the efficiency of DSSCs and other energy conversion technologies.

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CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

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