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Simulation of the CDs/TiO_2 Sample Behavior and Analysis of Its Curve Variations via SCAPS

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Abstract

The development of low-cost and environmentally friendly solar cell technologies has attracted significant attention as an alternative to traditional silicon-based devices. Carbon dots (CDs), owing to their tunable optical band gap, strong absorption in the visible spectrum, and excellent electron-donating properties, have emerged as promising sensitizers and interfacial modifiers in solar energy conversion systems. In this study, we present a systematic investigation of CDs/TiO_2 heterojunction solar cells using both experimental findings reported in the literature and numerical simulations performed with SCAPS-1D. The structural configuration consists of a transparent conducting oxide (TCO), a TiO_2 electron transport layer, a CDs absorber, and metallic contacts. Current density-voltage (J-V) characteristics were obtained to evaluate photovoltaic performance. The results demonstrate a short-circuit current density (Jsc) of approximately 16.518 mA/cm^2, an open-circuit voltage (V_{OC}) of about 0.772 V, a fill factor (FF) of 51.44 %, and a power conversion efficiency (PCE) approaching 6.56%. These values are consistent with experimental studies, validating the potential of CDs as efficient light harvesters. Furthermore, the role of interfacial defects and contact properties was analyzed, highlighting the importance of interface engineering to minimize recombination losses.

Subject Areas

Material Experiment

Keywords

Carbon Dots, TiO_2, Solar Cells, SCAPS Simulation, J-V Characteristics, Solar Cells

1. Introduction

The rapid depletion of fossil fuels and the global demand for clean energy have intensified research into photovoltaic devices with high efficiency and low cost. Among emerging materials, titanium dioxide (TiO_2) has been widely employed as an electron transport layer due to its stability, non-toxicity, and favorable band alignment [1]. However, the wide band gap of TiO_2 (~3.2 eV) restricts its ability to absorb visible light, thereby limiting its efficiency as a sole photo-absorber. Advanced elements such as titanium and carbon are central to modern clean energy technologies, particularly in dye-sensitized solar cells (DSSCs). Combining TiO_2 and CDs enhances energy conversion efficiency, reduces environmental costs, and aligns with Saudi Arabia's Vision 2030, supporting large-scale projects like NEOM and King Abdullah City for Atomic and Renewable Energy [2] [3]. Carbon dots (CDs) are unique nanomaterials with broad-spectrum light absorption, strong photoluminescence, and electron transport facilitation, while being environmentally friendly and less toxic than conventional metallic dyes [4]. Their tunable surface allows local production in Saudi Arabia, fostering innovation and R&D jobs within Vision 2030.

TiO_2 efficiently conducts electrons in solar cells, featuring chemical and thermal stability, with surface modification extending visible light absorption, supporting high-performance local solar materials development. Challenges such as limited light absorption and electron mobility can be overcome through optimized nanolayer design and integration with CDs, leading to more efficient solar cells and smart plants capable of low-light operation, supporting sustainability and clean energy objectives under Vision 2030. Carbon dots (CDs), a new class of carbon-based nanomaterials, exhibit excellent photoluminescence, high quantum yield, and tunable band gaps depending on synthesis routes. CDs can act as light sensitizers to extend the absorption spectrum of TiO_2 into the visible region, as well as passivate surface defects at interfaces, thereby reducing recombination. Previous studies have reported that CDs/TiO_2 composites enhance photoinduced charge transfer and significantly improve photovoltaic performance.

Many scientific studies of research on titanium and carbon were done, which show the importance of these samples. Hao Wang (2016) demonstrated that integrating nitrogen-doped carbon dots (N-doped CDs) with TiO_2 enhanced visible light absorption and increased the energy conversion efficiency to 0.79% [5]. Meanwhile, Hongguang Li and Keyang Yin developed a simple in situ growth method for carbon quantum dots on the surface of TiO_2, achieving an efficiency of 0.87%, the highest among dye-sensitized solar cells [6]. Shi *et al.* (2016) confirmed that the presence of CQDs in the TiO_2 layer enhances electron diffusion and transfer rate, thereby improving photovoltaic efficiency [4]. Expanded the light absorption range from UV to visible, leading to increased current density and higher power conversion efficiency (PCE) [4]. Then N-CQD/TiO_2 enhanced solar cells achieved a conversion efficiency of 9.29%, about 10% higher than that of unmodified cells [4]. So, Dong *et al.* (2019) designed a layered TiO_2-CQD-TiO_2

structure that increased conversion efficiency by 28% compared with pure TiO_2 [3]. In 2023, Tung, Imae, Huang, and Yadeta (2023). Used a CQDs/TiO_2 layer in solar cells, increasing the efficiency from 14.52% to 17.58% while improving stability and reducing defects [7]. And Li, Shi, Huang, Yang, and others (UCLA & Huazhong) developed a CQDs/TiO_2 electron transport layer, raising the cell efficiency to 19% due to improved charge transport and reduced recombination losses [8]. All studies confirmed that integrating carbon quantum dots (CQDs) with TiO_2 improves light absorption, electron transport, stability, and overall solar cell efficiency [3]-[8].

This work aims to explore the photovoltaic characteristics of a CDs/TiO_2 heterojunction solar cell structure, emphasizing the current density-voltage (J-V) response and its correlation with interfacial and material parameters. Here we have studied simulation of the CDs/TiO_2 sample behavior and analysis of its curve variations via SCAPS and its role in enhancing solar cell performance and sample preparation method CDs/TiO_2 and study at room temperature (300 K), then analysis at different temperatures. The integration of TiO_2 and CDs provides a solid foundation for future energy technologies, delivering high efficiency, low cost, and environmental sustainability, fully aligned with Vision 2030's goal of building a green, innovative, and sustainable economy. The significance of this sample is aligned with the Kingdom of Saudi Arabia's Vision 2030, which emphasizes reducing energy consumption and increasing reliance on renewable energy sources. This study contributes to advancing solar energy technologies by utilizing the prepared sample to enhance the efficiency and sustainability of solar cells.

2. Materials and Methods

2.1. Simulation Parameters

SCAPS (Solar Cell Capacitance Simulator) is a one-dimensional solar cell simulation program developed at Ghent University, Belgium, within the Department of Electronics and Information Systems (ELIS). It is widely used for the design, modeling, and optimization of solar cells and is free for researchers and scholars in the field of photovoltaic energy [9] [10]. With the ability to simulate up to seven semiconductor layers, SCAPS enables the examination of many types of solar cells, including CIS, CdTe, Si, GaAs, and a-Si. The software computes important properties, including current-voltage (J-V), capacitance-voltage (C-V), and quantum efficiency (QE), and integrates recombination mechanisms like SRH, Auger, and band-to-band. In photovoltaic research, SCAPS is an essential instrument that facilitates the design and improvement of solar cell efficiency as well as the examination of how internal structure and physical parameters impact device performance.

SCAPS-1D software was used to model device performance. Parameters such as band gap, electron affinity, dielectric permittivity, effective density of states, electron/hole mobility, and interface defect density were extracted from published literature. Interface recombination was included to evaluate its effect on efficiency.

The SCAPS-1D simulation framework is based on the numerical solution of the

one-dimensional semiconductor equations (Drift-Diffusion Model) [10] [11]. These equations form the mathematical foundation for analyzing the steady-state performance of a solar cell.

- Poisson's Equation: This equation relates the spatial distribution of the electrostatic potential (ψ) to the total charge density (ρ) within the semiconductor material. It is essential for determining the internal electric field.

$$\frac{\partial}{\partial x}\left(\varepsilon_0 \varepsilon \frac{\partial \varphi}{\partial x}\right) = -q\left(p - n + N_D^+ - N_A^- + \frac{\rho_{def}}{q}\right) \tag{1}$$

- Continuity Equations: These equations express charge conservation and describe the balance between carrier generation (G), recombination (U), and current density (J_n, J_p):

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

$$\frac{1}{q}\frac{\mathrm{d}J_n}{\mathrm{d}x} = -G_{op}(x) - R(x) \tag{3}$$

2.2. Device Structure

The CDs/TiO_2 hybrid composite is a promising material for photocatalytic and optoelectronic applications because of its exceptional physicochemical features. Carbon quantum dots (CDs) greatly increase the light absorption range from the ultraviolet to the visible region when included in titanium dioxide (TiO_2), improving the efficiency of solar energy usage. Additionally, the CDs function as excellent electron mediators, effectively preventing photogenerated electron-hole pairs from recombining, hence increasing TiO_2's photocatalytic activity. The composite is appropriate for biomedical and environmental applications due to its strong chemical and thermal stability, non-toxicity, and environmental friendliness. Furthermore, CDs improve TiO_2's electrical conductivity, which speeds up charge transfer during photoelectrochemical reactions. Because of its straightforward synthesis methods and adjustable structure. Furthermore, CDs improve TiO_2's electrical conductivity, which speeds up charge transfer during photoelectrochemical reactions. The CDs/TiO_2 composite has a lot of potential for use in solar energy conversion, hydrogen production, and pollutant degradation because of its easy synthesis methods and adjustable structural and surface characteristics.

The individual solar cell structures used for the simulation have been shown in **Figure 1**. The solar cell structure was designed with the higher ITO layer, followed by the CDs layer and the rest of the TiO_2 layer. The schematic representation of the structure used in the simulation has been shown in **Figure 2**.

To define each layer in the device model, material characteristics including thickness, bandgap, electron and hole carrier concentrations, and electron affinity are essential. The simulation's layer parameters are listed in **Table 1** [12] [13]. **Table 2** includes the layer and interface defect specifications, respectively.

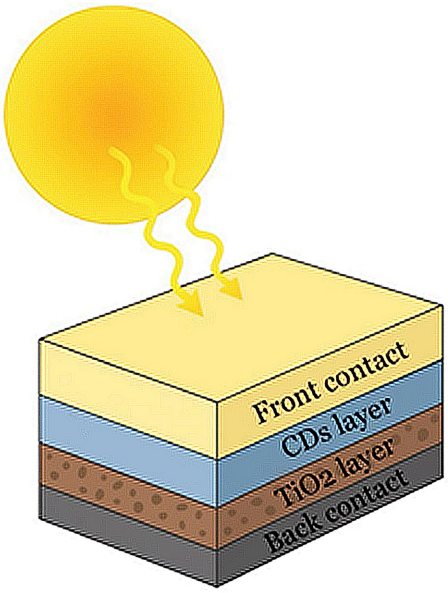

Figure 1. Device structure TiO_2 solar cell.

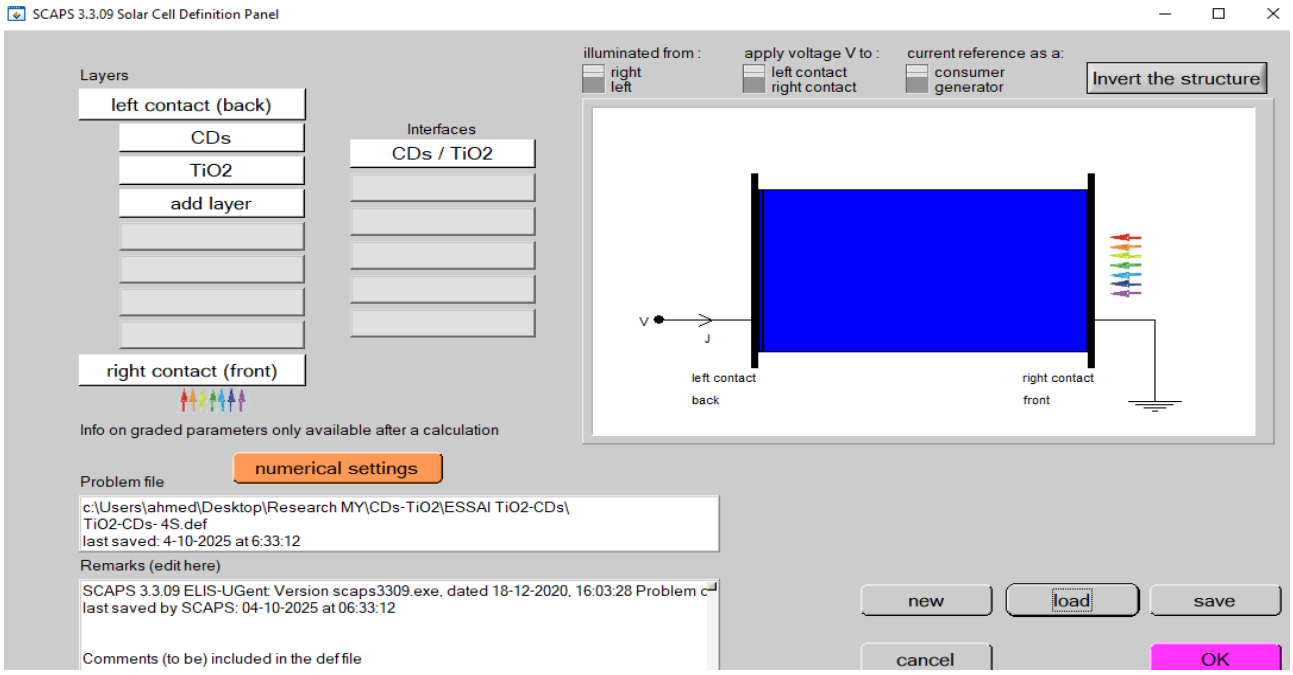

Figure 2. Device structure of simulated CDs/TiO_2 solar cell from SCAPS one-dimensional solar cell simulation program.

Defects are added to the absorber layers and are listed in **Table 2** [12] [14] in order to make experimental results realistic. Additionally, series resistance (Rs) of 1 Ωcm^2 and shunt resistance (Rsh) of 10 Ωcm^2 are the simulation parameters used throughout the tests. The AM 1.5 spectrum with an input power density of 1000 W/m^2 and a temperature of 300 K (room temperature) was used to set illumination circumstances that resemble normal reporting conditions, as shown in **Figure 1**. Furthermore, certain surface recombination characteristics were used for the simulated device's front and rear electrodes [15]. The front electrode has a metal

work function of 5.3 eV, an electron surface recombination velocity of 10^1 cm/s, and a hole surface recombination velocity of 10^1 cm/s. On the other hand, **Table 2** lists the metal work function [16] [17], electron surface recombination velocity, and hole surface recombination velocity of the back electrode as 5.1 eV, 107 cm/s, and 105 cm/s, respectively.

Table 1. The input parameters values used for SCAPS-1D in the simulation of the solar cell structure [12].

Parameters	CDs	TiO_2
Thickness	200	50
Band gap (E_g)	2.5	3.20
Electron affinity (χ)	3.8	4.00
Relative permittivity (ε_r)	6	50
N_c (CB effective DOS)	$10 * 10^{19}$	$2.0 * 10^{18}$
N_v (VB effective DOS)	$1.0 * 10^{19}$	$1.0 * 10^{19}$
Electron mobility μ_n	0.1	2.0
Hole mobility μ_p	0.01	0.01
Donor/acceptor doping	$1 * 10^{14}$	$1 * 10^{16}$

Table 2. Interface defects parameters in CDs/TiO_2 [12].

Parameters	CDs/TiO_2 Interface
Defect type	Neutral
Capture cross-section e^-s (cm^2)	1×10^{-15}
Capture cross-section h^+s (cm^2)	1×10^{-15}
Energetic distribution	Single
Reference for defect energy level (E□)	Mid-gap (Eg/2 of CDs)
Total defect ($1/cm^2$)	$\approx 1 \times 10^{12}$
IDL thickness (cm)	1×10^{-7}
Volumetric Nt (cm^{-3})	1×10^{19}

3. Results and Discussion

The solar cell performance was characterized in terms of J-V curves under AM1.5G illumination (100 mW/cm^2). Extracted parameters include V_{OC}, J_{SC}, *FF*, and PCE [18].

3.1. J-V Characteristics at Room Temperature

The J-V (current density-voltage) curve (**Figure 3**) represents the electrical performance of the simulated solar cell as obtained from SCAPS-1D under standard illumination conditions (AM 1.5G, 1000 W/m^2, 300 K). This curve provides es-

sential information about the photovoltaic parameters and the overall device efficiency [18].

Under forward and reverse bias conditions, SCAPS calculates the current density (J) as a function of the applied voltage (V). From the resulting J-V curve, the key photovoltaic parameters are extracted:

- Open-circuit voltage (V_{OC}): The voltage at which the current density becomes zero ($J = 0$).
- Short-circuit current density (J_{SC}): The current density at zero applied voltage ($V = 0$).
- Fill factor (FF): Indicates the "squareness" of the J-V curve and is calculated as:

$$FF = \frac{J_{mp} \times V_{mp}}{V_{OC} \times J_{SC}} \tag{4}$$

where J_{mp} and V_{mp} are the current density and voltage at the maximum power point (MPP).

- Power conversion efficiency (PCE η): The ratio of the output electrical power to the incident light power, expressed as

$$\eta = \frac{V_{OC} \times J_{SC} \times FF}{P_{in}} \tag{5}$$

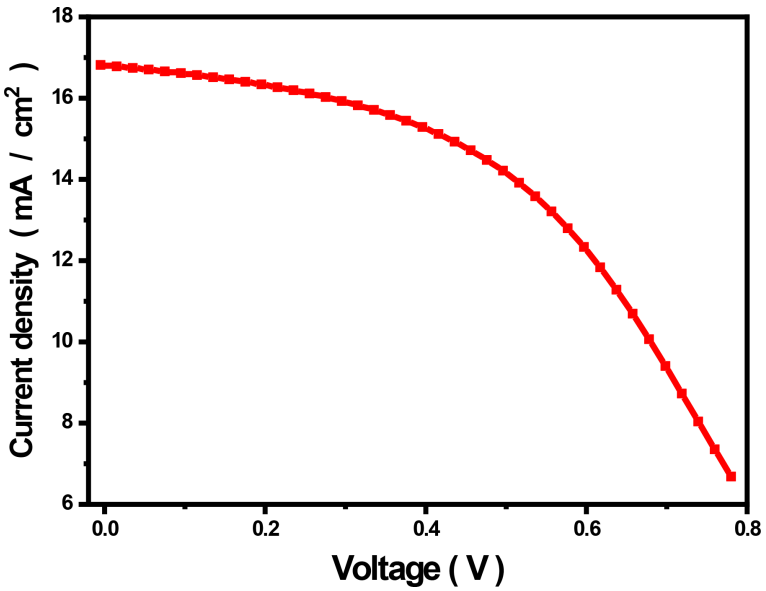

Figure 3. Short-circuit current density J_{SC} vs. voltage (V) curves for solar cells.

The shape of the J-V curve (**Figure 3**) reflects the quality of the junction and the recombination mechanisms within the device. A well-behaved J-V curve shows a sharp knee near the maximum power point, indicating low series resistance and efficient carrier extraction. The curve's shape reflects the quality of the interlayer connection and the recombination mechanisms within the cell; a steep curve near the maximum power point indicates low series resistance and

efficient carrier extraction. From this curve, key photovoltaic parameters can be determined, such as open-circuit voltage (V_{OC}), short-circuit current density (J_{SC}), fill factor (FF), and photovoltaic conversion efficiency (PCE (η)).

The simulated J-V curve showed typical diode-like behavior with a photocurrent plateau under illumination. These curves were analyzed under simulated one sun. The device exhibited an excellent average PCE (η) of 6.56% with a short circuit current density (J_{SC}) of 16.518 mA/cm^2, an open circuit voltage (V_{OC}) = 0.772 V, and a fill factor (FF = 51.44%). The value of the filling factor is related to several physical effects that affect the internal resistors, recombination rates, and p-n junction characteristics within the solar cell.

These values are in good agreement with experimental reports of CDs/TiO_2 solar cells, which typically achieve efficiencies in the range of 1% - 8% depending on synthesis method and interface quality [19].

Figure 4 represents the quantum efficiency (QE) curve for CDs/TiO_2-based solar cells using SCAPS software, at room temperature. This curve represents the variations of the quantum efficiency as a function of wavelength from 0 to 600 nm.

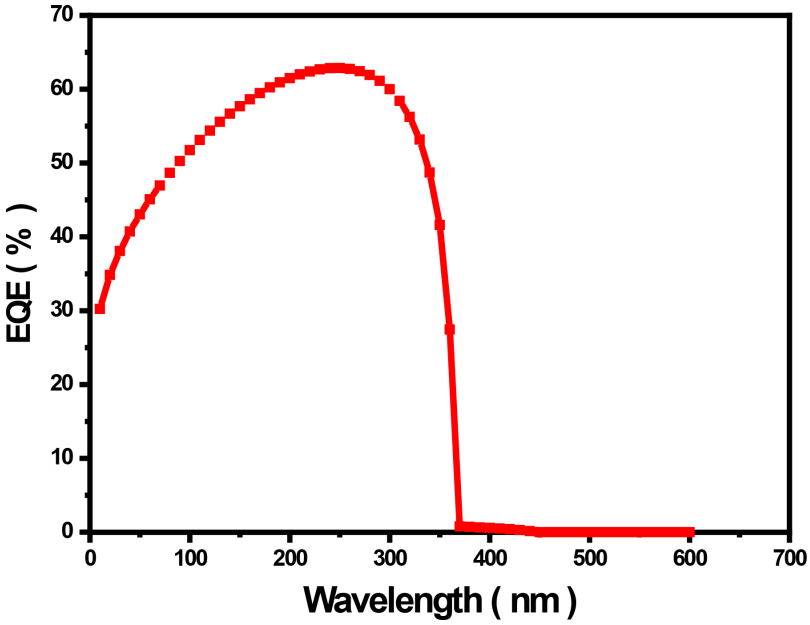

Figure 4. Simulation EQE (%) vs. Wavelength (nm) curves for solar cells.

3.2. Effect of Temperatures

Figure 5 shows the simulated current density (J_{SC} - Current Density - J) curve with voltage (V) for CDs/TiO_2-based solar cells at different temperatures using the SCAPS software. Changing the voltage from 0 V to 0.8 V yields different current densities (Current Density, J). Temperatures were varied from 100 K to 800 K to test the solar cell's performance.

The effect of temperature between CDs and TiO_2 was found to play a critical role in recombination dynamics. As temperature increases, the short-circuit current density (J_{SC}) of CDs/TiO_2 composites changes due to variations in carrier

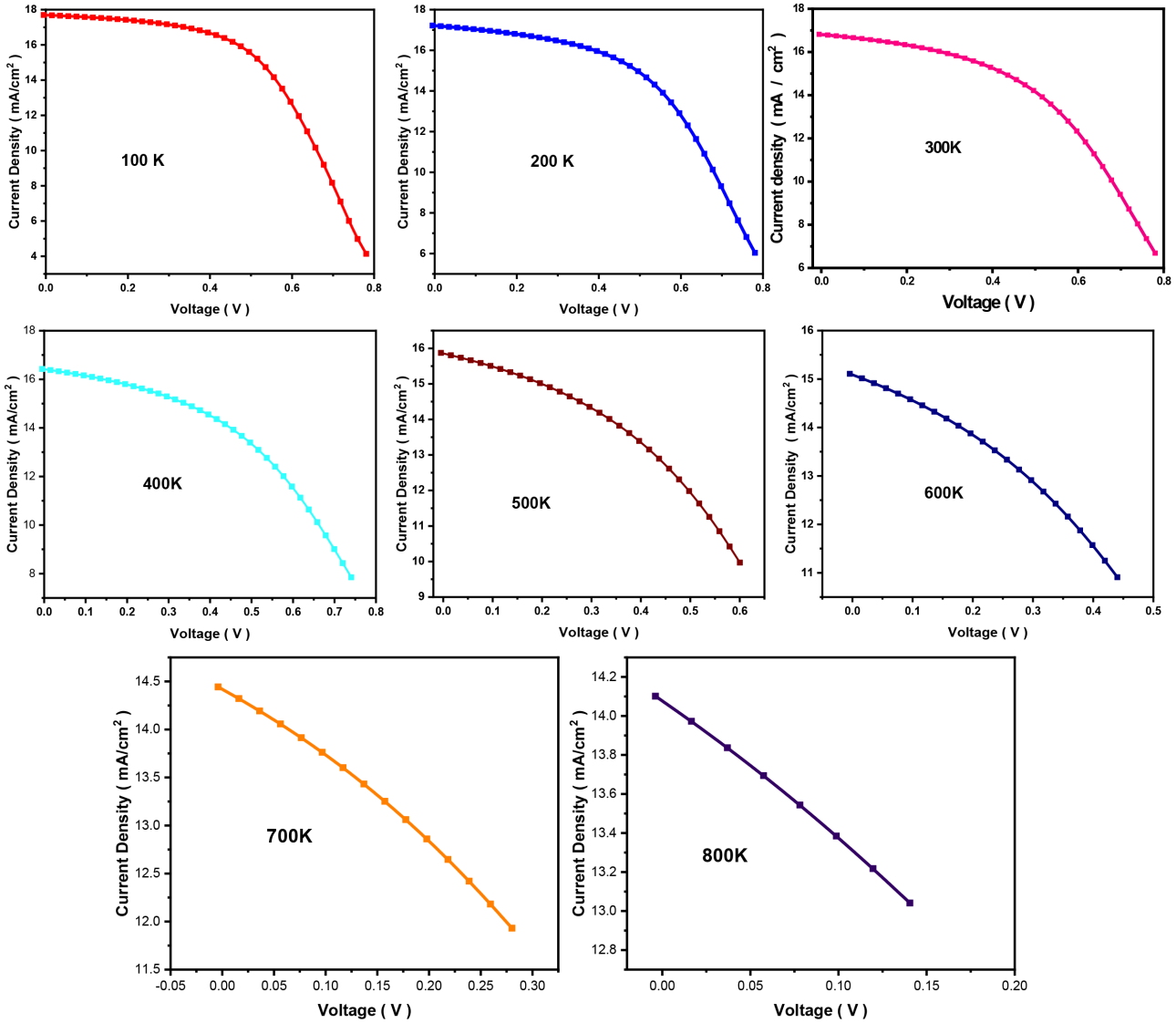

Figure 5. The effect of temperature on the simulated current density (J_{SC}) versus voltage (V) curves of CDs/TiO_2-based solar cells.

mobility and recombination rates. At low temperatures, the carrier mobility decreases, leading to a lower J_{SC}. While at high temperatures, a significant decline in J_{SC} appears because of enhanced recombination or partial material degradation. Moderate heating (up to 50˚C) enhances J_{SC} and QE by improving charge mobility and interface quality, while higher temperatures (>70˚C) induce recombination and reduce efficiency.

The Quantum Efficiency (QE) or Incident Photon-to-Current Efficiency (IPCE) increases significantly after incorporating carbon dots (CDs) into TiO_2. This enhancement broadens visible-light absorption (400 - 620 nm) and improves charge separation and interfacial stability, even under thermal stress. At moderate temperatures, improved carrier mobility and efficient charge transfer between CDs and TiO_2 dominate, enhancing both J_{SC} and QE. At higher temperatures, defect formation and recombination losses reduce the efficiency.

When the temperature increases, the open-circuit voltage decreases V_{oc} (Figure 6). Electrons gain more thermal energy, which increases the rate of recombination inside the cell. This reduces the potential difference between the two terminals, and V_{OC} decreases. The short-circuit current slightly decreases (J_{SC}) at the higher temperature, increasing thermal losses and electron recombination, which causes the generated current to drop slightly. In summary, when the temperature increases, the efficiency of the solar cell decreases because both V_{OC} and J_{sc} decrease.

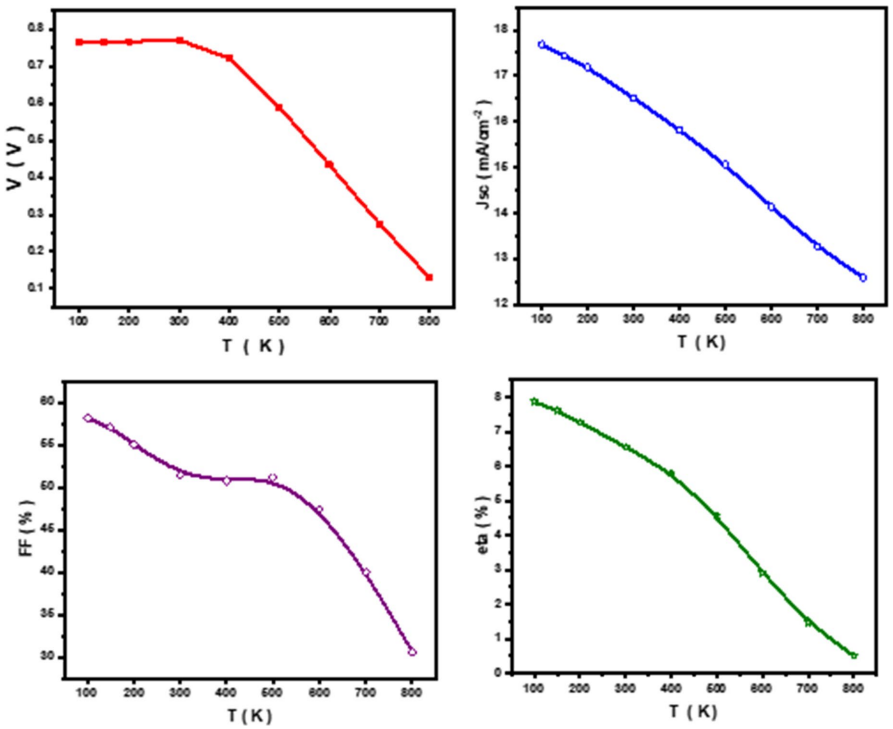

Figure 6. The impact of temperature on solar cell performance.

At high temperature, the efficiency (η) decreases (Figure 6). This is due to the increase in recombination at a lower open circuit voltage (V_{OC}), and at a high internal resistance. This augmentation of temperature causes the fullness factor (*FF*) to decrease, which is due to the increased serial resistance and the deterioration of the quality of communication between classes.

On the other hand, efficiency (η) increases when temperature (T) decreases (Figure 6). Because V_{OC} rises and decreases heat losses. In addition, the fullness factor (*FF*) changes because the internal resistance decreases. The decrease in the fill factor (*FF*) with increasing temperature is mainly attributed to the temperature-induced degradation of the electrical properties of the solar cell. As the temperature rises, the reverse saturation current increases significantly, leading to a noticeable reduction in V_{oc}. In addition, higher temperatures increase the series resistance and enhance carrier recombination, especially near the maximum power region. These combined effects reduce the squareness of the J-V curve and result in a lower *FF*.

This study shows that high defects reduced both V_{OC} and *FF*, while significantly

increasing efficiency (**Figure 6**). So, we demonstrate enhanced efficiency when CDs are incorporated into TiO_2-based solar cells, supporting the other results [20] [21]. The synergy between CDs and TiO_2 lies in improved visible-light absorption and efficient charge transfer across the heterojunction.

4. Conclusion

The potential of CDs/TiO_2 solar cells as an affordable and sustainable photovoltaic technology is highlighted in this study. The efficiency of the solar cell declines as the temperature rises because both V_{OC} and Jsc drop. Furthermore, a decrease in internal resistance causes a change in the fullness factor (*FF*). According to simulation results, CDs can efficiently increase charge transfer and prolong light absorption, improving J-V performance. Carbon quantum dots were added to titanium dioxide to greatly enhance the solar cells' ability to capture light and carry charges. Increased photoelectric conversion was the outcome of the two materials' synergy, demonstrating that CQDs are a promising addition for improving TiO_2-based solar systems. Future research should concentrate on improving synthesis techniques. This will lower the density of interfacial defects and investigate different back connections to increase device efficiency.

Conflicts of Interest

The authors declare no conflicts of interest.

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