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Simulation of P-CdTe and N-TiO₂ Heterojunction Solar Cell Efficiency

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Abstract

The present study presents a numerical analysis of p-type CdTe and n-type TiO₂ heterojunction solar cells. The simulations were conducted using SCAPS-1D software to investigate the effects of varying the thickness of the p-type CdTe layer, the temperature, and the band gap on the efficiency of the solar cell. The results show that the efficiency of the solar cell increases from 16.81% to 18.28% as the thickness of the p-type CdTe layer is varied from 1.0 to 5.0 μm and decreases from 17.95% to 11.67% as the temperature is varied from 300 to 400 K. The efficiency also increases from 15.29% to 19.26% as the band gap is varied from 1.40 to 1.55 eV. For the p-CdTe/n-TiO₂ heterojunction solar cell, the optimized absorber layer thickness is 3 μm , and the optimized temperature and band gap are 300 K and 1.5 eV, respectively. At these optimized parameters, the highest efficiency (PCE) achieved was 17.95%, with a V_{OC} of 0.766 V, J_{SC} of 27.75 mA/cm^2 , and FF of 84.39%. These results provide theoretical guidelines for fabricating efficient p-CdTe/n-TiO₂ heterojunction solar cells.

Keywords: Heterojunction; Numerical Simulation; Photovoltaic Solar Cell; SCAPS Software

1 Introduction

Energy and the environment are two critical and interrelated topics, and using non-renewable energy sources such as oil, coal, and gas contributes to environmental degradation [1]. The need for sustainable energy has led to the development of various experimental procedures for synthesizing and depositing metal oxides to improve solar cell efficiency [2]. However, numerical simulation provides a cost-effective approach to improving solar cell efficiency without requiring extensive lab work and expenses [3]. Metal oxides have unique mechanical and electrical properties, making them easy to synthesize and design, and they are eco-friendly and have a wide band gap [4]. In this study, we investigate the effect of varying the thickness of p-type CdTe, temperature, and band gap on the efficiency of n-type TiO₂ and p-CdTe heterojunction solar cells using Solar Cell Capacitance Simulator (SCAPS-1D) software. The thickness of the absorber layer is a crucial factor in solar cells as it directly affects cell performance [5]. TiO₂ has a direct band gap of 3.2 eV to 3.35 eV, making it n-type and suitable for heterojunctions with most p-type materials [6]. CdTe, on the other hand, is a chalcogenide material with a direct band gap of 1.5 eV and a high absorption coefficient, making it a popular choice for use in solar cells due to its high efficiency, low cost, and long-term stability [7].

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The current study builds on previous work on p-CdTe and n-TiO₂ heterojunctions by investigating the photoelectrical properties of the device and the charge transport mechanism at the interface of the n-TiO₂/p-CdTe heterojunction [8]. The study also considers the effect of thickness variation on device performance. Reduced series resistance and improved shunt resistance led to a high fill factor and enhanced device performance [9]. The thickness of the absorber layer also affects the light-trapping phenomenon at the interface of the semiconductor junction, which directly impacts solar cell efficiency [10], [11]. In addition, surface roughness can affect solar cell efficiency, and therefore, the study also investigates the effect of temperature variation on device performance [12]. In this study, we use SCAPS-1D software to simulate a metal oxide/metal chalcogenide heterojunction device and investigate the effects of thickness, temperature, and band gap on device performance. We record the performance results and aim to enhance the efficiency of the solar cell. Simulations are run using the SCAPS-1D software at AM1.5G [1 sun] lamp illumination. The efficiency of heterojunction solar cell is significantly affected by thickness and band gap of photoactive material, and temperature of the cell. Thus, the effects of variation in the thickness and band gap of CdTe, and temperature of a cell on the device performance were investigated.

2 Methodology

2.1 SCAPS-1D software

The SCAPS-1D software, which was designed by the Department of Electronics and Information Systems (ELIS) at the University of Gent, Belgium [13], was used to simulate the DC and AC electrical characteristics of the thin film heterojunction. This software can numerically fabricate solar cells by adding up to seven layers and is based on semiconducting equations such as Poisson's and continuity equations [14].

2.2 Simulation setup

The simulation was performed using SCAPS-1D software version 3310. The default Left and Right contacts were used, and optoelectrical parameters of every heterojunction layer were input parameters for the simulation. The software provides results and graphs for open circuit voltage (V_{OC}), short circuit current density (J_{SC}), fill factor (FF), and quantum efficiency (QE%) [14].

2.3 Simulation parameters

The material parameters for the heterojunction's window and absorber layers were collected precisely from authentic literature [14]. These input material parameters, including Band gap (Eg) eV, Electron affinity (χ) eV, Relative dielectric permittivity (ϵ_r), Electron mobility (μ_e) cm²/V.s, Hole mobility (μ_h) cm²/V.s, Effective density state in C.B. (N_C) cm⁻³, Effective density state in V.B. (N_V) cm⁻³, Acceptor density (N_A) cm⁻³, Donor density (N_D) cm⁻³, were used for calculations. Table 1 shows the specific material parameters used in this study.

Table 1: Parameters for simulation modeling of (n-TiO₂/p-CdTe)-based thin film solar cells.

Material parameter	n-TiO ₂	p-CdTe
Thickness (μm)	0.5	1.0
Band gap (eV)	3.1	1.5
Electron affinity (χ)	4.2	3.9
Relative dielectric permittivity	10	9.4
CB effective density of states (1/cm ³)	2.00E+17	8.00E+17
VB effective density of states (1/cm ³)	6.00E+17	1.80E+19

2.3.1 Parametric optimization and evaluation

The theoretical analysis of the n-TiO₂/p-CdTe heterojunction was performed using SCAPS-1D software under AM1.5 G, 100 mW/cm² illumination ranges. The "set absorption model" and "absorption file" modes were chosen for each heterojunction layer to perform the simulation. The heterojunction's default back and front contacts were set, and the standard solar spectrum of AM1.5 G was used for illumination [14]. The heterojunction solar cell was optimized by varying the thickness of the p-CdTe absorber layer and the temperature of the heterojunction. The simulation results for J_{SC} , V_{OC} , η , and FF of the designed heterojunction were obtained.

Figure 1 (a) shows the schematic presentation of the n-TiO₂/p-CdTe heterojunction, while Figure 1 (b) shows the energy band diagram of n-TiO₂/p-CdTe solar cells. The energy band diagram was used to study the properties of the heterojunction solar cells. Table 2 shows the back and front contact parameters and the working temperature. The band alignment between the absorber layer (p-CdTe) and the window layer (n-TiO₂) is crucial as it affects current transmission across the heterojunction interface and the performance of thin films. The energy band alignment shows that the p-CdTe absorber layer (Eg = 1.5 eV) and n-TiO₂ window layer

($E_g = 3.1$ eV) have an excellent band diagram with each other, which can lead to high conversion efficiency for absorbed photons with energy nearly equal to or greater than a band gap of 1.5 eV.

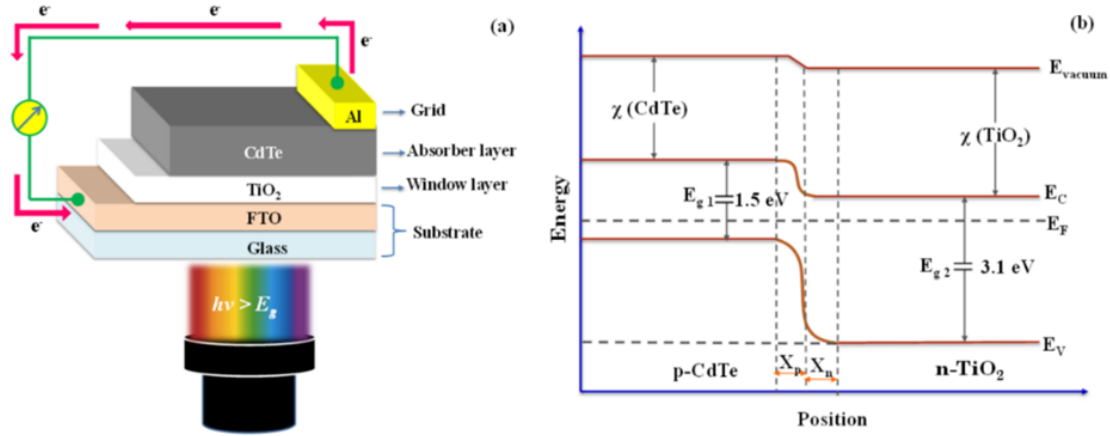


Figure 1: (a) Schematic diagram of the n-TiO₂/p-CdTe heterojunction solar cell and (b) schematic band energy diagram of the n-TiO₂/p-CdTe heterojunction.

Table 2: Parameters of the front and back contact used in the simulation of the (n-TiO₂/p-CdTe) solar cell.

Parameter	Back contact electrical properties	Front contact electrical properties
Surface recombination velocity of electrons (cm/s)	10^5	10^2
Surface recombination velocity of holes (cm/s)	10^7	10^5
Work function (eV)	4.98	4.09
Working temperature (K)	300K	

3 Results and Discussion

3.1 Effect of variation in the thickness of the absorber layer (p-CdTe) on cell performance

In a p-CdTe/n-TiO₂ heterojunction, the window layer typically has a lower thickness than the absorber layer to support fast exciton transport with a low recombination rate, resulting in a high current generation and maximum absorption at high voltages. In this study, the thickness variation effect of the p-CdTe layer on the heterojunction performance was investigated by varying the thickness of the p-CdTe layer from 1 to 5 μm with an interval of 1 μm while keeping the thickness of the n-TiO₂ layer fixed at 0.5 μm . The input parameters of the heterojunction are reported in Table 1. The impact of the p-CdTe thickness variation on the J-V curve, quantum efficiency, V_{OC} , J_{SC} , FF, and PCE were studied. As shown in Table 3, V_{OC} slightly increased from 0.751 to 0.773 V, and J_{SC} increased from 26.35 to 28.13 mA/cm^2 with the increase in p-CdTe thickness. The PCE also increased from 16.81 to 18.28 %, while FF decreased from 84.91 to 84.28 %. The optimal thickness for the p-CdTe absorber layer was found to be 3 μm , where the efficiency increased by 0.57 %. After 3 μm the increase in efficiency is just by value of 0.2 %, indicating that a thickness greater than 3 μm was unnecessary for device fabrication. The increase in thickness of the p-CdTe layer led to the absorption of more photons, resulting in an increase in current [4], [15].

Table 3: Effect of the thickness of the absorber layer (CdTe) on the cell efficiency parameters.

Thickness (μm)	J_{SC} (mA/cm^2)	V_{OC} (V)	JMMP (mA/cm^2)	VMM (V)	FF%	$\eta\%$
1.0	26.35	0.751	25.39	0.662	84.91	16.81
2.0	27.39	0.760	26.33	0.668	84.51	17.60
3.0	27.75	0.766	26.72	0.671	84.39	17.95
4.0	27.97	0.770	26.94	0.673	84.18	18.15
5.0	28.13	0.773	27.10	0.674	84.28	18.28

Furthermore, the higher thickness of p-CdTe resulted in a lower recombination rate of excitons, allowing them more time to move before recombination. This, in turn, resulted in combined excitons that did not drop their energy as proximately upon hitting the absorber layer, leading to the observed increase in PCE. However, at higher thicknesses, excitons in the p-CdTe layer can undergo Auger recombination, transferring their energy to existing electrons and holes and reducing efficiency [16], [17], [18].

The band energy diagram of the optimized heterojunction n-TiO₂/p-CdTe indicates that hole recombination is more probable in the valence band of CdTe, while electron recombination is more probable in the conduction band of TiO₂. Increasing the thickness of the p-CdTe layer leads to an enhancement in quantum efficiency up to 3 μm, beyond which the quantum efficiency saturates. The numerical simulation results suggest that 3.0 μm is the optimal thickness for the p-CdTe layer. Figure 2 (a-f) illustrates the J-V, QE%, V_{OC}, J_{SC}, FF, and PCE curves for variations in the thickness of the given heterojunction solar cell.

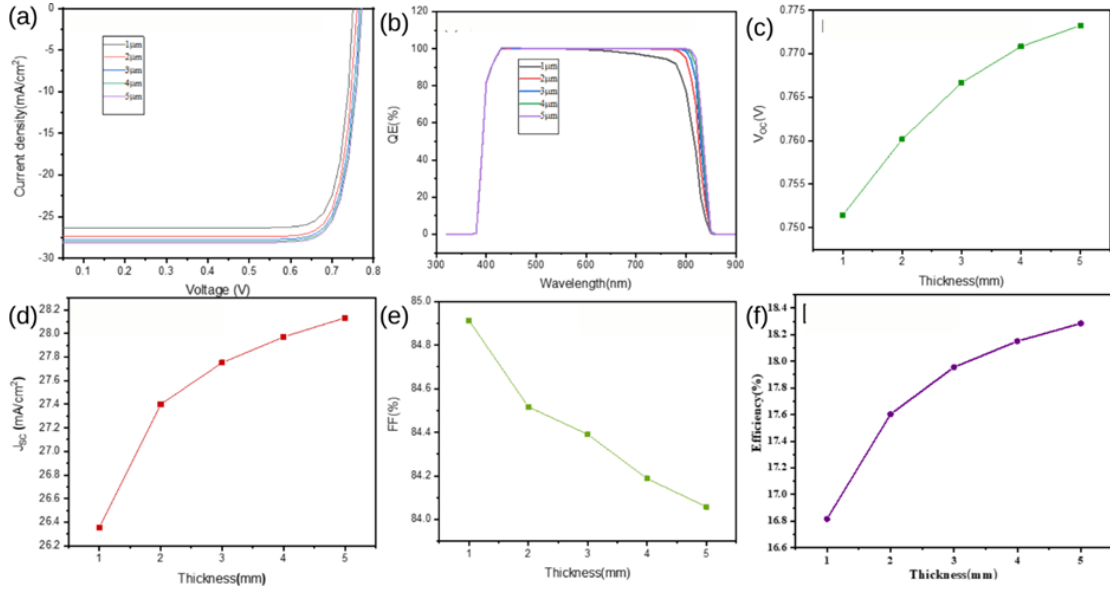


Figure 2: (a) Current-voltage (J-V) curves; (b) quantum efficiency (QE) as a function of wavelength; (c) open-circuit voltage (V_{OC}); (d) short-circuit current (J_{SC}); (e) fill factor (FF); (f) efficiency curves of the TiO₂/CdTe heterojunction at various thicknesses

3.2 Effect of variation of temperature on cell performance

The study of the temperature-dependence behavior of solar cells is crucial since the temperature has a contrary effect on the performance of heterojunctions. Different types of solar cells exhibit varying responses to temperature, with thin film solar cells being less sensitive to temperature than crystalline silicon solar cells. Additionally, the aging of the active layer affects the temperature coefficient of polymer solar cells, and the substrate temperature, reaction processing temperature, and annealing temperature can affect solar cell performance. As solar cells are exposed to various temperature ranges in different applications, monitoring the solar cell performance by varying the temperature range is important. In this work, we varied the temperature between 300 and 400 K and monitored the solar cell performance under optimized conditions. The results obtained under the optimized conditions are shown in Table 4, and the J-V curve for the effect of temperature variation on J-V, QE %, V_{OC}, J_{SC}, FF, and PCE was studied and reported in Figure 3 (a-f). An increase in temperature is beneficial for solar cell outcomes as it causes an increase in charge carriers; however, it limits to a certain extent because increased temperature affects the transport of charge carriers [19], [20]. As the temperature increases, the V_{OC} of the solar cell decreases, resulting in a decrease in cell efficiency.

Table 4: Effect of the thickness of the absorber layer (CdTe) on the cell efficiency parameters.

Temperature (K)	J _{SC} (mA/cm ²)	V _{OC} (V)	JMMP (mA/cm ²)	VMM (V)	FF%	η%
300	27.75	0.766	26.72	0.671	84.39	17.95
320	28.10	0.740	26.94	0.643	83.21	17.33
340	28.10	0.713	26.85	0.614	82.29	16.51
360	28.10	0.686	26.66	0.587	81.15	15.65
380	28.14	0.571	26.34	0.474	77.61	12.49
400	28.15	0.544	26.08	0.447	76.67	11.67

At the same time, an increase in temperature causes a slight increase in J_{SC}, which reduces the band gap energy with an increase in operating temperature. Thus, overall efficiency depends on the cooperation between a reduction in V_{OC} and an increase in J_{SC}. The results show that by varying the temperature from 300 to 400 K with an increment of 20 K for each interval, there was a significant decrease in V_{OC} from 0.766 to 0.544 V, FF from 84.39 to 76.07 %, and PCE from 17.95 to 11.67 %, but the J_{SC} value showed a slight increase from 27.75 to 28.15 mA/cm². The highest efficiency of 17.95 % was obtained at 300 K, and the efficiency decreased as the temperature increased. Therefore, 300 K is the optimized temperature for the n-TiO₂/p-CdTe heterojunction. When the operating temperature of heterojunction solar cells increases, the carrier concentration also increases, causing an increase in the rate of internal exciton recombination [21], [22]. This leads to an increase in the reverse saturation current, ultimately resulting in a decrease in V_{OC} (0.766 to 0.544) V.

At the same time, increased temperature causes a decrease in the band gap, which is responsible for a small increase in J_{SC} (27.75 to 28.15) mA/cm^2 . However, as the temperature increases, thermally active photons cause the scattering of charge carriers, affecting material conduction and decreasing heterojunction efficiency [23].

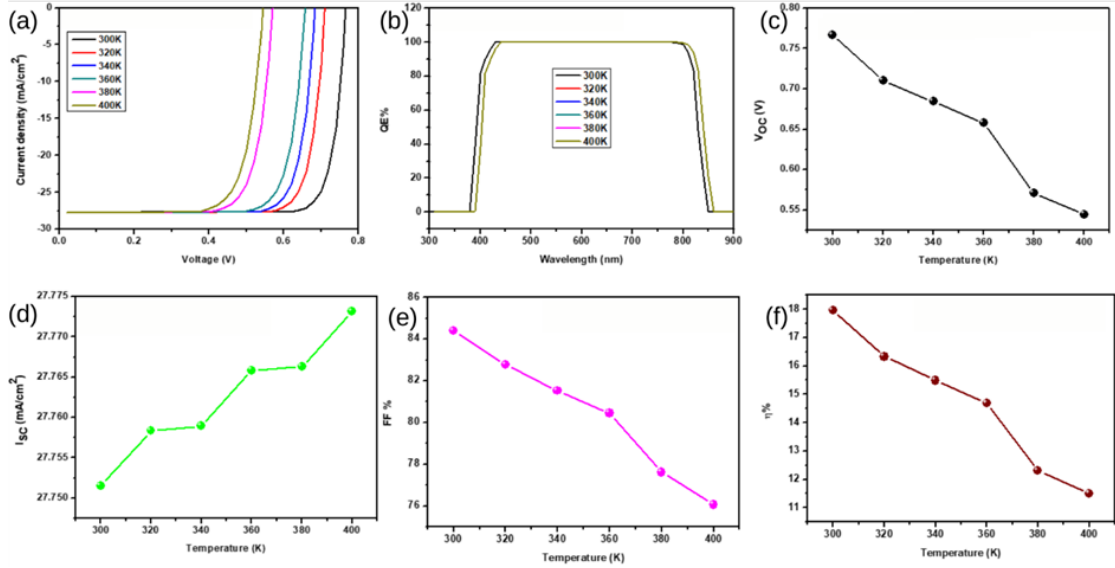


Figure 3: (a) Current-voltage (J - V) curves; (b) quantum efficiency (QE) as a function of wavelength; (c) open-circuit voltage (V_{OC}); (d) short-circuit current (J_{SC}); (e) fill factor (FF); (f) efficiency curves of the TiO_2/CdTe heterojunction at various temperatures.

3.3 Effect of band gap variation of absorber layer (p-CdTe) solar cell performance

The band gap is a crucial factor that affects the conversion performance of solar cells. Photons with energy nearly equal to the band gap energy participate in the photovoltaic effect [24], [25]. While each material has a fixed band gap, it can change when the semiconductor device is disturbed by external energy such as photons, electrical and magnetic fields, temperature, and pressure. The band gap is temperature-dependent; as the band gap of the material increases, its temperature dependency decreases. The band gap reflects the bond energy of the atom, and as the temperature increases, atomic vibrations increase, causing electrons to travel from the VB to the CB. Consequently, the band gap of the material decreases with increasing temperature [26]. When light falls on the window layer of the heterojunction, only those photons having energy nearly equal to the band gap energy show a transition from the VB to CB [27]. This determines the limit of the maximum wavelength of the solar spectrum, and absorption of this wavelength results in power production.

Table 5: Effect of the thickness of the absorber layer (CdTe) on the cell efficiency parameters.

Band gap (eV)	J_{SC} (mA/cm^2)	V_{OC} (V)	JMMP (mA/cm^2)	VMM (V)	FF%	$\eta\%$
1.40	27.758	0.666	25.59	0.575	82.64	15.29
1.45	27.757	0.716	26.64	0.623	83.43	16.60
1.50	27.751	0.766	26.72	0.671	84.39	17.95
1.55	27.750	0.829	26.80	0.718	84.70	19.26

The photovoltaic effect will not occur when the band gap is too high. For low band gap materials, excess photonic energy is wasted after partial utilization to excite electrons to overcome the bandgap [28]. In this study, the band gap of p-CdTe was varied between 1.40 and 1.55 eV while keeping the window layer band gap constant. The simulation results are shown in Figure 4 (a-f), and the corresponding values of V_{OC} , J_{SC} , FF, and efficiency are listed in Table 5. The band gap of a material has a direct impact on the ejection and absorption of photons, and it varies with the material. The band gap of the material is also correlated with the thickness of the p-CdTe layer, which decreases with increasing thickness. The band gap of the p-CdTe material plays a vital role in enhancing the photovoltaic properties, absorption ability, and lifetime of carriers [29], [30], [31]. The impact of band gap alteration on the PCE of modulated heterojunctions was investigated in this work. The results showed that increasing the band gap of the absorber layer between 1.40 and 1.55 eV led to an increase in PCE from 15.29 to 19.26 % with a slight decrease in current density. The highest efficiency of 17.95 % was achieved at a band gap of 1.5 eV. After conversion failure occurred at a band gap of 1.55 eV, the optimized band gap for the n- $\text{TiO}_2/\text{p-CdTe}$ solar cell was determined to be 1.5 eV.

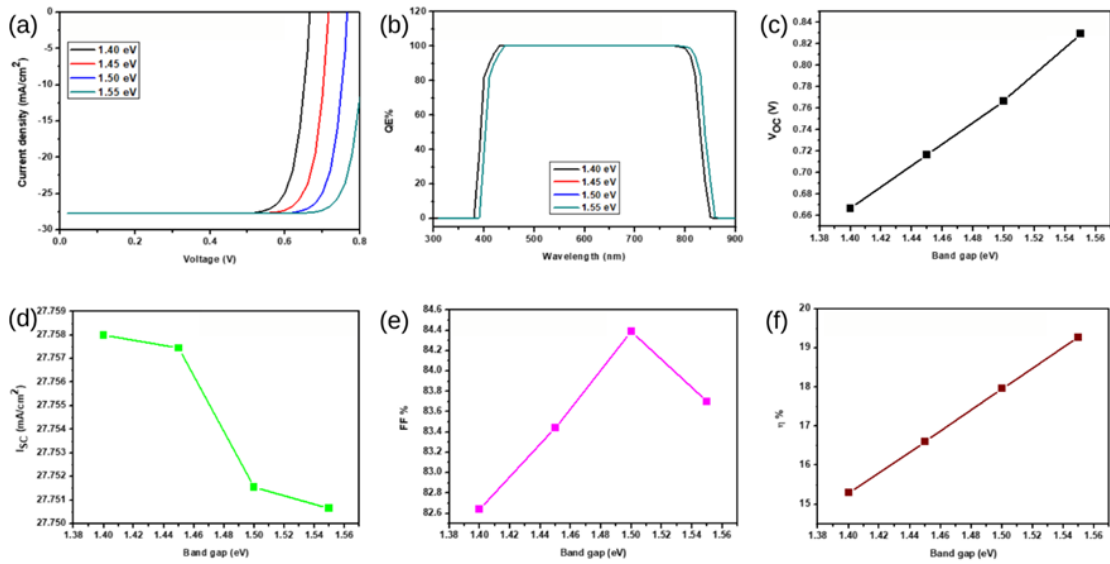


Figure 4: (a) Current-voltage (J-V) curves; (b) quantum efficiency (QE) as a function of wavelength; (c) open-circuit voltage (V_{OC}); (d) short-circuit current (J_{SC}); (e) fill factor (FF); (f) efficiency curves of the TiO_2/CdTe heterojunction concerning band gap variations.

3.4 Simulation at optimized parameters

To optimize the performance of the p-CdTe/n- TiO_2 heterojunction solar cell, a series of simulations were conducted to determine the optimal values of temperature, thickness, and band gap. Temperature significantly affects the performance of a solar cell by influencing carrier mobility, diffusion length, and carrier recombination rates. After conducting simulations at different temperatures, it was found that the optimal temperature for this solar cell was 300 K, which is approximately room temperature. The thickness of the absorber layer, p-CdTe, also affects the performance of the solar cell. If the layer is too thin, it may not absorb sufficient photons, while a layer that is too thick may result in more carrier recombination. After conducting several simulations, an optimal thickness of 3 μm was determined for this solar cell. The band gap of the absorber layer was varied between 1.40 eV and 1.55 eV, while the band gap of the window layer was kept constant. The simulations revealed that the optimal band gap for this solar cell was 1.5 eV. A band gap that is too high can result in insufficient photon absorption, while a band gap that is too low can lead to excessive recombination and a reduced open-circuit voltage. After determining the optimal values for temperature, thickness, and band gap, a simulation was carried out under these conditions to evaluate the performance of the solar cell. The simulation yielded a power conversion efficiency (PCE) of 17.95 %, which is the highest achieved for this solar cell. This was accompanied by a V_{OC} of 0.766 V, a J_{SC} of 27.75 mA/cm^2 , and a fill factor (FF) of 84.39 %.

Table 6: Simulation results of the p-CdTe/n- TiO_2 heterojunction solar cell under optimized conditions.

Optimized parameters	J_{SC} (mA/cm^2)	V_{OC} (V)	JMMP (mA/cm^2)	VMM (V)	FF%	$\eta\%$
Temperature 300K						
Thickness 3 μm	27.75	0.766	26.72	0.671	84.39	17.95
Band gap 1.5eV						

These values indicate efficient conversion of incoming photons to electrical energy and transport of carriers through the device. The results of this simulation are illustrated in Figure 5 (a) and Figure 5 (b), and the corresponding values are presented in Table 6.

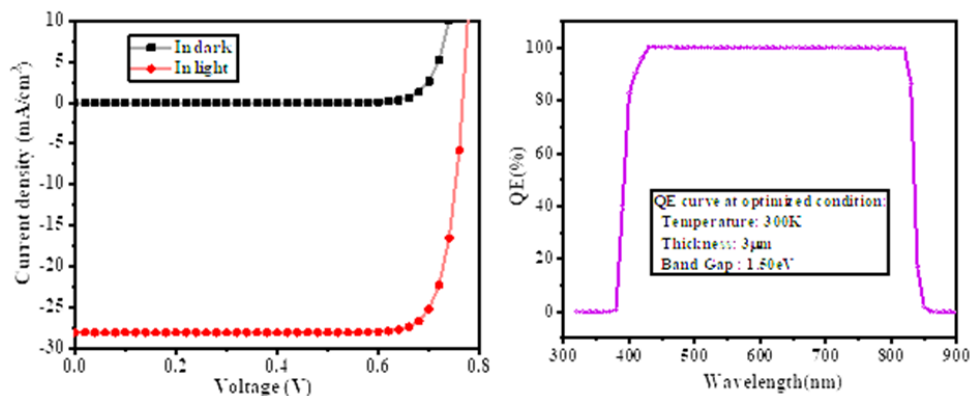


Figure 5: (a) Current-voltage (J-V) in the dark and in light and (b) quantum efficiency (QE) of the optimized solar cell simulation.

4 Conclusion

The present study utilized a simulation approach to examine the electrical and physical properties of a p-CdTe/n-TiO₂ heterojunction using SCAPS-1D software. The proposed p-CdTe/n-TiO₂ heterojunction solar cell was studied by varying the band gap, thickness, and temperature while keeping all electrical parameters constant. The simulation results showed that the optimized values of temperature, thickness, and band gap are 300 K, 3.0 μm, and 1.50 eV, respectively. Under these conditions, the highest power conversion efficiency (PCE) of 17.95 % was achieved with a V_{OC} of 0.766 V, J_{SC} of 27.75 mA/cm², and FF of 84.39 %. The obtained results indicate that the proposed p-CdTe/n-TiO₂ heterojunction solar cell exhibits the best performance under the optimized conditions. This theoretical modeling approach provides important guidelines for the fabrication of cost-effective thin-film solar cells. The findings of this study contribute to the development of efficient and sustainable photovoltaic devices with potential applications in the field of renewable energy.

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Declaration of Competing Interests

The author declares that she has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Funding Declaration

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Author Contribution

Akanksha S. Chougale: Conceptualization, Methodology, Writing - Original draft preparation, Writing - Reviewing; **Harshad D. Shelke:** Conceptualization, Visualization, Investigation, Methodology, Data curation; **Bikram Prasad:** Conceptualization, Visualization, Investigation, Methodology, Data curation; **Sandesh R. Jadhkar:** Investigation, Methodology, Data curation; **Nithesh Naik:** Investigation, Methodology, Data curation; **Habib M. Pathan:** Supervision, Methodology, Writing - Reviewing; **Dnyaneshwar R. Shinde:** Supervision, Methodology, Writing - Reviewing.

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