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Optimizing Electron Diffusion, Temperature, and Photoanode Thickness for Enhanced Photovoltaic Efficiency in TiO_2/CuS Dye-Sensitized Solar Cells (DSSCs)

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Abstract

This study addresses a critical gap in optimizing electron diffusion, operational temperature, and photoanode thickness to enhance the photovoltaic efficiency of TiO_2/CuS-doped dye-sensitized solar cells (DSSCs). While previous studies have investigated individual parameters affecting DSSC performance, limited research examines their combined effects on charge transport and recombination rates. Through computational modeling, we evaluated photoanode thicknesses from 1 μm to 100 μm and operational temperatures from 260 K to 350 K, analyzing their influence on electron mobility, recombination rates, and overall efficiency. Results show that the electron diffusion coefficient increases with temperature, reaching a maximum of 1.626×10^{-6} cm^2/s at 350 K, thereby enhancing electron transport and reducing recombination losses. An optimal photoanode thickness of 3 μm was identified, yielding the highest efficiency of 17.28% across the temperature range. Efficiency declines at thicknesses exceeding 3 μm due to extended electron diffusion paths and higher recombination rates. These findings underscore the importance of balancing temperature and structural parameters to improve charge transport and minimize losses, particularly for DSSC applications in warm environments.

Introduction

Solar energy is one of the most promising alternatives to fossil fuels, with Earth receiving approximately 1,200,000 TW of solar energy annually, far exceeding the global energy requirement of about 20 TW [1], [2]. Among various solar technologies, dye-sensitized solar cells (DSSCs) have gained significant attention due to their low-cost materials, ease of fabrication, and potential for large-scale production [3], [4]. However, despite these advantages, DSSCs have yet to achieve the efficiency levels required for widespread commercialization. Optimizing their power conversion efficiency (PCE) is thus essential, primarily through advancements in material selection and structural components [5]–[7].

The TiO_2 photoanode is a critical component in DSSCs, facilitating electron transport and influencing overall performance [8], [9]. Doping TiO_2 with copper sulfide (CuS) has shown potential in enhancing electron mobility and reducing recombination losses, which are crucial for improving PCE [10]. Nonetheless, while material improvements contribute to performance gains, comprehensive optimization of operational parameters—such as electron diffusion, temperature, and photoanode thickness—is necessary to leverage TiO_2/CuS-based DSSCs' potential fully. Prior research underscores that parameters like photoanode thickness and operating temperature directly impact electron mobility and recombination rates, both of which are vital for improving charge transport and minimizing energy losses [8], [11]–[13].

Despite advancements, the interaction between temperature and photoanode thickness in enhancing DSSC performance remains underexplored, particularly for TiO_2/CuS-doped systems. While these factors have been studied independently, their combined effect on optimizing electron diffusion and charge transport has not been adequately addressed. Temperature influences electron mobility, while photoanode thickness affects light absorption and electron transport efficiency. How these two parameters interact could significantly impact the overall efficiency of DSSCs, but this relationship has not been fully examined in the context of TiO_2/CuS-based systems. Investigating their interaction is crucial, as it can reveal opportunities for synergistic improvements that would not be apparent when considering each factor in isolation.

This study aims to systematically investigate the effects of electron diffusion, temperature, and photoanode thickness on DSSC performance, focusing on the conditions that optimize photovoltaic efficiency. Specifically, the study seeks to (1) identify the operational temperature that maximizes electron mobility while minimizing recombination, (2) determine the optimal photoanode thickness to balance light absorption and electron transport, and (3) provide guidance for DSSC design suitable for fluctuating temperature environments.

This research addresses a critical gap in the field by exploring the combined optimization of these parameters—350 K operational temperature and a 3 µm photoanode thickness—to increase efficiency in TiO_2/CuS-doped DSSCs. While prior studies have focused on individual parameters, the integrated approach presented here provides new insights into how parameter combinations can enhance DSSC performance. The findings will support the development of high-efficiency DSSCs tailored for warm environments, where temperature control and optimized structural parameters are essential for achieving stable, high performance.

Theory and Calculation

Temperature Dependence

The electron diffusion coefficient, D was modeled as temperature-dependent functions [14], [15]:

$$D = \frac{kT\mu}{q} \tag{1}$$

where k is the *Boltzmann's constant*, T is the temperature, is μ the electron mobility, and q is the electron charge. This model assumes that electron mobility increases with temperature, a behavior observed in experimental studies of TiO_2-based DSSCs. The parameter values were chosen based on literature, with mobility (μ) values taken from previous work on CuS-doped TiO_2 photoanodes to reflect realistic charge transport mechanisms at various temperatures.

J-V Characteristics

For each combination of photoanode thickness and temperature, the J-V characteristics were simulated using the following equation for the *short-circuit* current density (Jsc) [14], [15]:

$$J_{SC} = \frac{q\Phi La}{1-L^2a^2}\left[-La + \tanh\left(\frac{d}{L}\right) + \frac{La\exp(-da)}{\cosh\left(\frac{d}{L}\right)}\right] \tag{2}$$

where Φ is the photon flux, L is the diffusion length electron, a is the absorption coefficient, and d is the photoanode thickness. The *open-circuit* voltage (Voc) was determined from [14], [15]:

$$V_{OC} = \frac{kTm}{q}\ln\left[\left(\frac{LJ_{SC}}{qDn_0\tanh\left(\frac{d}{L}\right)}\right) + 1\right] \tag{3}$$

where m is the ideal factor and n_0 is the concentration of electrons in the dark. The model assumes uniform illumination and an ideal photon absorption factor, aligning with standard conditions used in DSSC simulations.

Optimization of Thickness and Temperature

The simulation results were analyzed to identify the optimal photoanode thickness and temperature combination that maximizes efficiency. For each simulated condition, the efficiency was calculated using the equation [14], [15]:

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

$$\eta = \frac{V_{OC}J_{SC}FF}{P_{in}} \times 100\ \% \tag{5}$$

where FF is the *fill factor*, J_{max} is the maximum power point current density, V_{max} is the maximum power point voltage, η is the efficiency, and P_{in} is the input power.

Simulation Method

This study employs computational modelling to optimize the electron diffusion coefficient, operational temperature, and photoanode thickness in TiO_2/CuS-doped dye-sensitized solar cells (DSSCs). The model integrates parameters such as the electron diffusion coefficient, temperature dependence, and recombination rate to evaluate their effects on electron mobility, recombination rates, and overall DSSC efficiency. Electron mobility (μ) values and recombination rates were sourced from previous studies on TiO_2/CuS photoanodes to ensure the model's accuracy, reflecting real-world charge transport mechanisms at varying temperatures. MATLAB R2022a software was used to conduct the simulation, providing flexibility to incorporate complex parameter interactions.

Assumptions and Justifications

The model assumes temperature primarily affects electron mobility and diffusion coefficient, impacting recombination rates and overall efficiency. Simulation results were compared to experimental data from similar studies on TiO_2/CuS-based DSSCs to validate the model. For instance, the optimal photoanode thickness of 3 μm aligns with findings from previous research, and the temperature-dependence of electron diffusion matches experimental observations as Equation (1): electron diffusion coefficient *(D)*, Equation (2): *short-circuit* current density (Jsc), Equation (3): *open-circuit* voltage (Voc).

The thickness of the TiO_2/CuS photoanode was varied from 1 μm to 100 μm to investigate its impact on electron transport and light absorption. The optimal thickness was identified based on balancing maximizing light absorption and minimizing recombination losses. The thickness of 3 μm was found to be optimal based on a combination of experimental studies and simulation results that suggest this thickness enhances both electron mobility and light capture efficiency without excessively increasing recombination as Equation (4): *fill factor* (FF) and Equation (5): efficiency (η).

Simulation Conditions

The simulation was conducted under varying operational temperatures (260 K to 350 K) to explore how temperature influences electron diffusion and recombination rates. It is assumed that the temperature primarily affects the electron mobility and diffusion coefficient, influencing recombination rates. The selected temperature range (260 K to 350 K) reflects practical operational conditions for DSSCs, particularly in warm environments with expected temperature fluctuations. A 10-degree increment was chosen to capture gradual changes in electron diffusion without excessive computational demand, addressing the need for efficient yet detailed data representation. The simulation also examined the effects of varying photoanode thickness on electron transport and light absorption, confirming the optimal thickness of 3 μm based on enhanced electron mobility and minimized recombination rates. MATLAB R2022a software implemented the model and simulated the J-V characteristics for each photoanode thickness and temperature combination. The internal parameters (Table 1) used in the simulation, including the electron mobility, absorption coefficient, and diffusion length, were derived from experimentally validated data sources to ensure the model's reliability in predicting real-world behavior.

Table 1. Internal Parameter Simulation.

Parameter	Mark	Information	References
$\boldsymbol{k}$	1.381×10^{-23} J/K	Boltzmann's constant	[12], [16]
$\boldsymbol{q}$	1.602×10^{-19} C	Payload electron	[12], [16]
$\boldsymbol{L}$	2.2361×10^{-3} cm	Diffusion length electron	[12], [16], [17]
$\boldsymbol{a}$	5000 cm^{-1}	Coefficient Absorption	[12], [14], [16], [17]
$\boldsymbol{m}$	4.5	Ideal factor	[12], [14], [16]–[18]
$\boldsymbol{\mu}$	5.39×10^{-3} m^2 V^{-1} s^{-1}	Mobility electron	[19]
$\boldsymbol{n_0}$	10^{16} cm^{-3}	Concentration electrons in dark	[12], [14], [16]–[18]
$\boldsymbol{d_{optimum}}$	3 $\boldsymbol{\mu}$m	Optimum thickness	[10]
$\boldsymbol{\Phi}$	1×10^{17} cm^{-2} s^{-1}	Intensity light sun	[12], [14], [16], [18]

Model Validation

The model assumes temperature primarily affects electron mobility and diffusion coefficient, impacting recombination rates and overall efficiency. Simulation results were compared to experimental data from similar studies on TiO_2/CuS-based DSSCs to validate the model. For instance, the optimal photoanode thickness of 3 μm aligns with findings from previous research, and the temperature-dependence of electron diffusion matches experimental observations.

Results and Discussion

This study uses computational modeling to investigate the optimization of electron diffusion, operational temperature, and photoanode thickness in TiO_2/CuS-doped dye-sensitized solar cells (DSSCs). The effects of varying these parameters on electron mobility, recombination rate, and charge transport efficiency were systematically analyzed across thicknesses from 1 μm to 100 μm and temperatures from 260 K to 350 K.

The simulation results in Fig. 1 show how increasing temperature affects *short-circuit* current density (Jsc) and *open-circuit* voltage (Voc) at the optimal photoanode thickness of 3 μm. These findings align with Lee et al.'s observations that optimal heating of TiO_2 improves electron transport properties by increasing electron mobility and minimizing recombination rates [8]. As temperature rises, electron mobility and diffusion increase, which decreases recombination probability and thereby boosts charge transport efficiency. This temperature-dependent increase in electron diffusion underlines the significance of temperature control in DSSCs, particularly for applications in warm environments. However, further temperature increases could compromise photoanode stability, suggesting an operational limit near 350 K, as the results indicate that both Jsc and Voc increase with temperature.

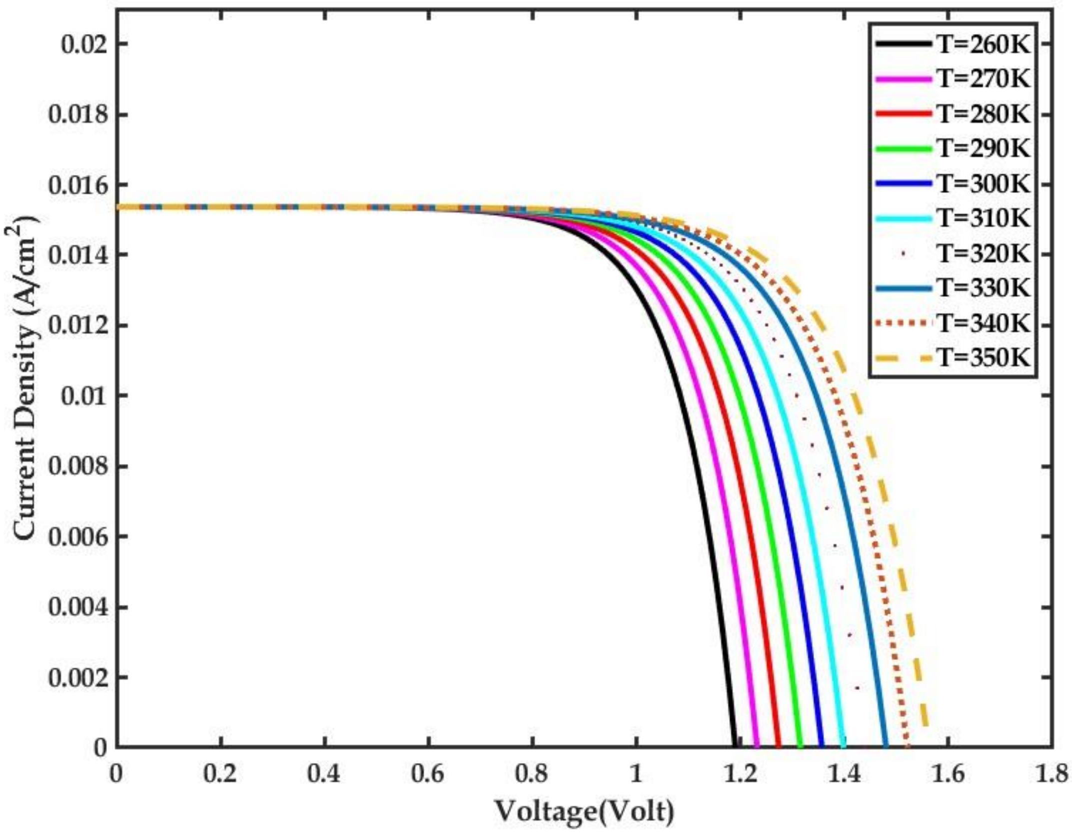

Figure 1. J-V Characteristics of TiO_2/CuS Photoanode DSSC as a Function of Temperature at Optimum Photoanode Thickness

The plot highlights that as temperature increases, both Jsc and Voc exhibit a consistent upward trend, peaking at 350 K. At this temperature, the DSSC achieves its maximum efficiency = 17.28% with Jsc = 15.37 mA/cm^2, Voc = 1.56Volt, and a *fill factor* (FF) of 0.72 (Table 2), which is attributed to the enhanced electron diffusion and reduced recombination losses. These results confirm that higher temperatures improve electron mobility, resulting in better charge transport. The simulation data (Table 2) reveal that the CuS-doped TiO_2 photoanode exhibits the highest efficiency and maximum power output (Pmax). This underscores the essential role of CuS in boosting electron transport and photon absorption efficiency [20].

Table 2. Data Results Simulation of TiO_2/CuS Photoanode DSSC at Optimum Thickness.

T (K)	$d_{optimum}$ (μm)	Jsc (mA/cm2)	Voc (Volt)	P_{max} (mA/cm² V)	FF	Efficiency (%)	References
260	3	15.37	1.19	13.25	0.72	13.25	[10]
270	3	15.37	1.23	13.71	0.72	13.71	
280	3	15.37	1.27	14.16	0.72	14.16	
290	3	15.37	1.32	14.61	0.72	14.61	
300	3	15.37	1.36	15.06	0.72	15.06	
310	3	15.37	1.40	15.51	0.72	15.51	
320	3	15.37	1.44	15.95	0.72	15.95	
330	3	15.37	1.48	16.40	0.72	16.40	
340	3	15.37	1.52	16.84	0.72	16.84	
350	3	15.37	1.56	17.28	0.72	17.28	

Table 2 summarizes the efficiency data from simulations across different temperature and thickness combinations, indicating that the best performance is achieved at 350 K and 3 μm. This combination maximizes photovoltaic efficiency by balancing enhanced electron mobility (due to higher temperature) with efficient light absorption (achieved through optimal thickness). These results reinforce that both temperature and thickness must be carefully controlled to optimize DSSC performance, as excessive thickness can negate the mobility benefits achieved through temperature increases by increasing the likelihood of recombination.

The increase in efficiency at this thickness aligns with results from other studies, which similarly highlight the importance of optimizing photoanode thickness to strike the ideal balance between photon absorption and charge transport [21], [22]. The optimal thickness of the TiO_2/CuS photoanode was identified as 3 μm, striking a balance between light absorption and electron transport efficiency. The simulation data (Table 2) show that DSSCs achieve the highest conversion efficiency at this thickness across varying temperatures. This finding is consistent with previous research by Aboulouard et al. [11], which concluded that efficiency diminishes beyond a certain photoanode thickness (around 5 μm) due to increased electron recombination resulting from a longer diffusion path. Studies using TiO_2 as the photoanode material have demonstrated that an optimal thickness of around 3-5 μm enhances dye absorption and light utilization, improving power conversion efficiency (PCE). For instance, Suseno et al. reported that optimizing layer properties and thickness can significantly impact DSSC performance, especially when organic dyes are used [5].

The combined optimization of temperature and thickness offers insights into how DSSCs can be designed for stable, high-efficiency operation in varying environmental conditions. This study's findings emphasize that controlling both parameters is essential for developing DSSCs suited to real-world applications in fluctuating temperatures. Future research may further explore the role of CuS doping levels and alternative dopants to enhance electron transport while maintaining structural stability at elevated temperatures.

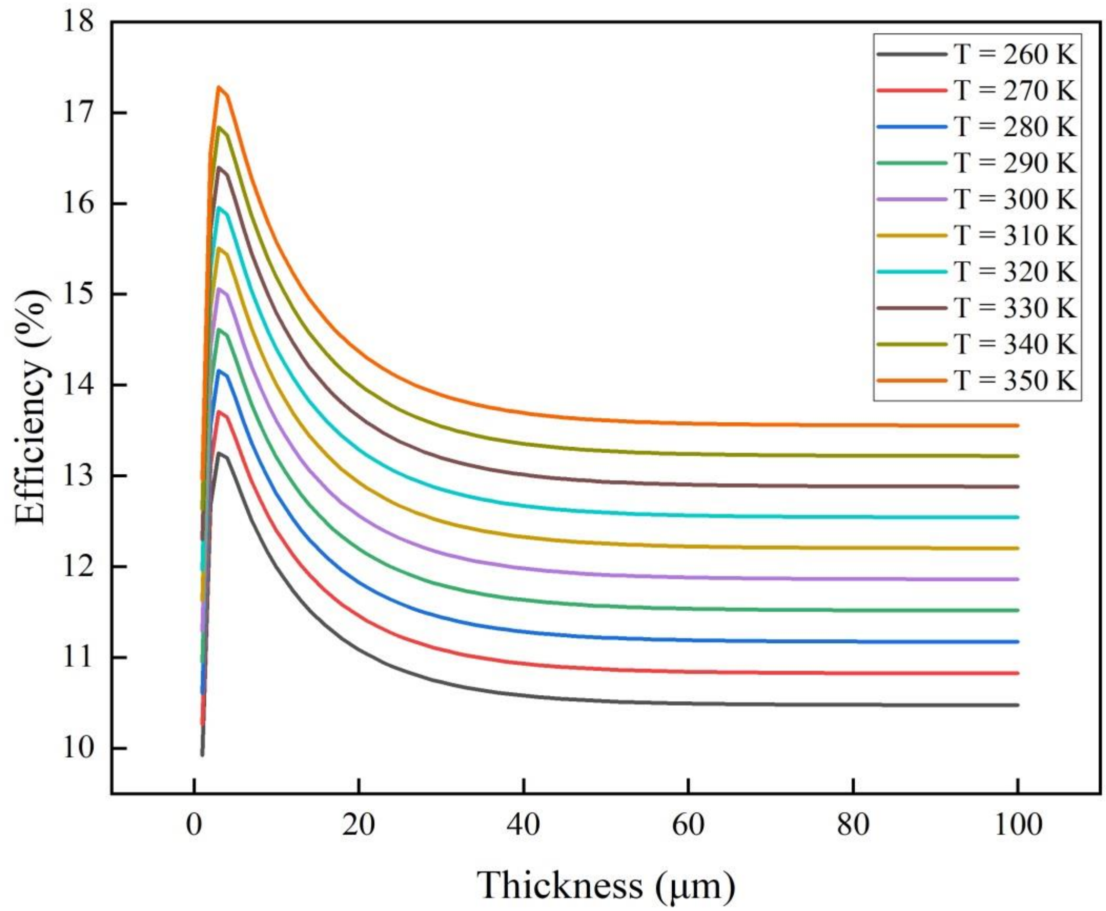

Figure 2. Relationship Between Photoanode Thickness and Efficiency Across Temperature Variations of TiO_2/CuS DSSC.

Figure 2 presents the effect of varying photoanode thickness on DSSC efficiency across the examined temperature range. The results indicate that a photoanode thickness of 3 μm consistently yields the highest efficiency across all temperatures, striking a balance between light absorption and minimized recombination. Thicknesses beyond 3 μm reduce efficiency due to prolonged electron diffusion paths, which increase recombination rates. These findings are consistent with prior research identifying 3-5 μm as the optimal thickness for balancing electron diffusion with light absorption in DSSCs [11].

The high efficiency at 3 μm is further enhanced by CuS doping, which provides additional electron transport pathways and increases electron mobility within the photoanode. This mechanism explains why CuS-doped TiO_2 exhibits improved electron transport and reduced recombination compared to undoped TiO_2, ultimately enhancing DSSC performance [10]. Similar studies, such as Aboulouard et al. [11], also observed diminishing returns on efficiency when photoanode thickness exceeded 5 μm, confirming that excessive thickness can hinder electron transport due to increased recombination losses.

The data from the simulation indicate that the electron diffusion coefficient (D) increases with temperature. As the temperature rises from 260 K to 350 K, the diffusion coefficient reaches a maximum of 1.626×10^{-6} cm^2/s. at 350 K (Table 3). This trend aligns with the findings of Lee et al. [8], who reported that annealing at optimal temperatures enhances electron transport properties in TiO_2 films, thereby reducing recombination losses, and the enhancement in electron mobility results in an increased diffusion coefficient (D), aligning with patterns observed in earlier research findings [23]. Also, this study underscores the significance of temperature regulation in enhancing DSSC performance, which is in line with earlier research demonstrating similar temperature-dependent efficiency patterns [24], [25].

Table 3. Data Results Simulation of Connection Operational Temperature and Electron Diffusion Coefficient of TiO_2/CuS Photoanode DSSC at Optimum Thickness.

T (K)	**$d_{optimum}$ (μm)**	**D (cm^2/s)**
260	3	1.208×10^{-6}
270	3	1.255×10^{-6}
280	3	1.301×10^{-6}
290	3	1.347×10^{-6}
300	3	1.394×10^{-6}
310	3	1.440×10^{-6}
320	3	1.487×10^{-6}
330	3	1.533×10^{-6}
340	3	1.580×10^{-6}
350	3	1.626×10^{-6}

The results (Table 3) indicate that the optimal operational temperature for maximizing DSSC performance is 350 K. At this temperature, the electron diffusion coefficient reaches its highest value, 1.626×10^{-6} cm^2/s, significantly improving electron transport and reducing recombination. Similarly, the optimal photoanode thickness of 3 μm consistently yields the best balance between light absorption and electron transport efficiency across all temperatures.

This increase in the electron diffusion coefficient is directly related to enhanced electron mobility (μ), which decreases the probability of recombination and improves cell efficiency. Equation 1 illustrates this dependency. Experimental evidence shows that higher temperatures enhance electron lifetime and mobility up to a threshold, after which structural integrity issues may arise [11].

To quantify the effect of temperature on DSSC performance, Figure 3 summarizes the electron diffusion coefficient (D) and power conversion efficiency (PCE) across all temperatures. This plot clearly illustrates the increasing trend of D with temperature, showing a significant enhancement in electron mobility as the temperature rises from 260 K to 350 K. The PCE also follows this trend, reaching a maximum of 350 K. However, it is essential to note that further temperature increases could potentially destabilize the photoanode structure, emphasizing the need for careful thermal management in practical applications.

By focusing on the relationship between temperature and performance metrics such as Jsc, Voc, D, and efficiency, this study demonstrates the critical importance of optimizing both operational temperature and photoanode thickness to enhance DSSC efficiency. This optimized combination of parameters provides a roadmap for future experimental studies to improve DSSC performance in real-world environments. The consolidated figures and comparative analysis presented in this section offer more precise insights into how temperature and thickness affect DSSC efficiency, addressing the limitations of the previous figure-heavy approach.

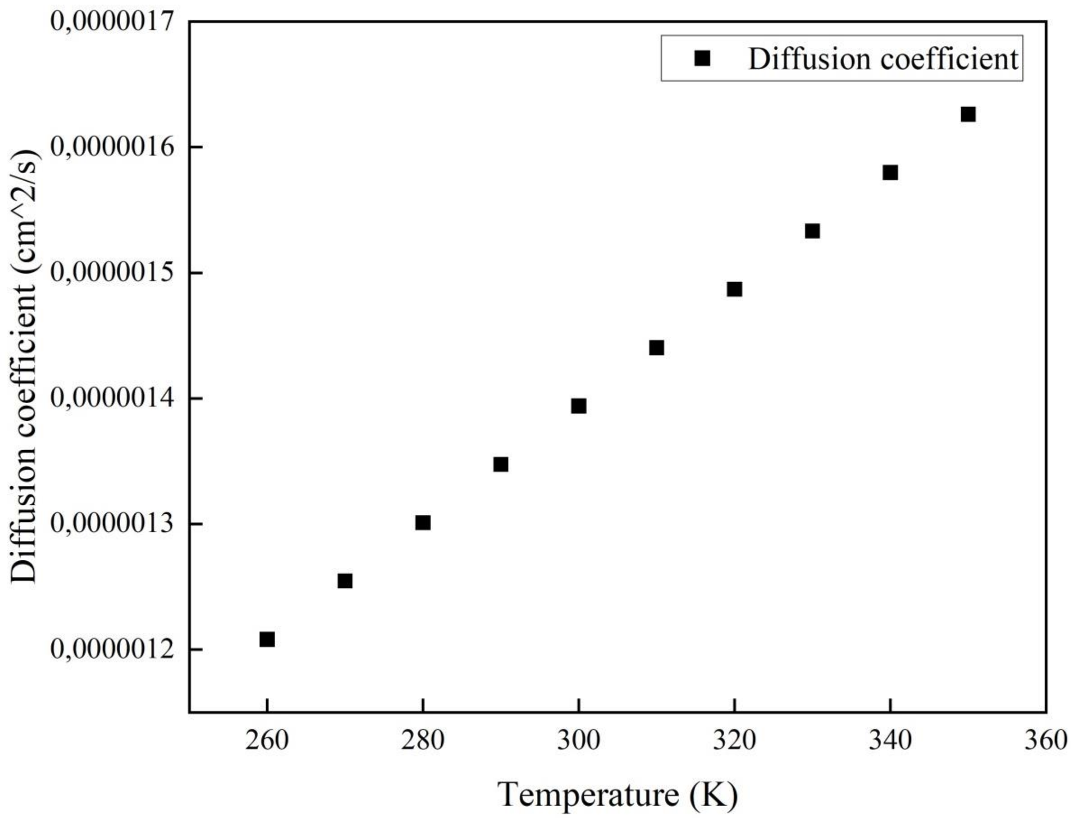

Figure 3. Electron Diffusion Coefficient and Efficiency Across Temperatures of TiO_2/CuS Photoanode DSSC at Optimum Thickness.

The relationship between operational temperature, electron diffusion coefficient, and efficiency is depicted in Figure 3. It illustrates that the electron diffusion coefficient increases with temperature, positively affecting efficiency. This result supports the findings of Aboulouard et al. [13], where a similar positive correlation between temperature and DSSC efficiency was observed. However, it is crucial to maintain the temperature within a range that does not compromise the structural integrity of the photoanode material.

Supriyanto et al. [10] investigated the effect of photoanode thickness and temperature, emphasizing the role of electron diffusion in determining the optimal conditions for DSSCs. The influence of different calcination temperatures on the crystallinity of TiO_2 nanoparticles and photoanode performance corroborates that thermal treatment significantly impacts efficiency [26]. The findings underscore the importance of controlling photoanode thickness and operational temperature to maximize DSSC efficiency. Doping TiO_2 with CuS improves the electron transport pathways, and optimizing the photoanode structure further enhances the cell's power conversion efficiency.

Conclusion

This study has systematically optimized operational temperature and photoanode thickness to enhance the photovoltaic efficiency of TiO_2/CuS-doped dye-sensitized solar cells (DSSCs). The results indicate that an operational temperature of 350 K and a photoanode thickness of 3 μm provide the optimal conditions for maximizing electron mobility and minimizing recombination losses, yielding an overall efficiency of 17.28%. These findings demonstrate that temperature increases up to 350 K significantly enhance electron diffusion, improving charge transport and reducing recombination. Similarly, the 3 μm thickness balances efficient light absorption and minimizes electron diffusion path length, reducing the likelihood of recombination.

The study's combined approach to optimizing temperature and photoanode thickness provides a practical set of parameters for designing high-efficiency DSSCs, particularly for warm environments where temperature management is crucial. However, it is important to recognize the limitations of using simulated data rather than direct experimental validation, and future studies should consider experimental testing to confirm the long-term stability of DSSCs under elevated operational temperatures.

Future research should explore the effects of further refining CuS doping levels and investigating alternative dopants that may provide enhanced electron transport while maintaining structural stability. These efforts will build on the current findings to support developing of DSSCs that are robust, efficient, and suitable for real-world applications in variable temperature conditions.

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