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APPLIED PHYSICS

Dye-sensitized solar cells (DSSC) have attracted significant research interest due to their semi-transparency, ease of fabrication, cost-effectiveness, and environmental friendliness. This research focuses on enhancing dye-sensitized solar cells efficiency by doping titanium dioxide with copper sulfide and varying internal parameters such as concentration, thickness, and temperature. The primary issue addressed is the low electron mobility of titanium dioxide, which limits its performance as a photoanode. Using simulation methods, this study analyzed dye-sensitized solar cells performance under different doping conditions. The results showed that the highest efficiency of 8.18 % was achieved at a TiO2/CuS concentration of 0.3 %. The optimal photoanode thickness was approximately 3 μm, yielding an efficiency of 8.33 %. Temperature variations at room temperature (275 K, 300 K, and 325 K) resulted in efficiency values of 13.94 %, 15.06 %, and 16.18 %, respectively. These findings indicate that targeted doping and precise control of internal parameters can significantly enhance the performance of titanium dioxidebased dye-sensitized solar cells. The improved efficiency is attributed to enhanced electron mobility and better structural and morphological characteristics of the doped titanium dioxide photoanode. This research provides valuable insights into developing more efficient and sustainable dye-sensitized solar cells. The practical implications of these results are significant for advancing dye-sensitized solar cells as a viable alternative to conventional solar cells, contributing to the global effort to address the energy crisis by providing a cost-effective and environmentally friendly energy source Keywords: photoanode, dye-sensitized solar cells, effi-

ciency, internal parameter variation, electron mobility

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OPTIMIZING DYE-SENSITIZED SOLAR CELL EFFICIENCY THROUGH TiO2/CuS DOPING: EFFECTS OF INTERNAL PARAMETER VARIATIONS

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1. Introduction

The global energy crisis, driven by the depletion of fossil fuel reserves and the increasing energy demand, necessitates the exploration of alternative energy sources. Dye-Sensitized Solar Cells (DSSCs) have emerged as a promising alternative to conventional solar cells due to their unique advantages, including semi-transparency, ease of fabrication, cost-effectiveness, and environmental friendliness. Since their introduction by Gratzel and O'Regan in 1991, DSSCs have attracted significant research interest for these reasons [1].

DSSCs typically consist of a photoanode made from a porous semiconductor, a dye, an electrolyte, and a conductive metal or carbon counter electrode. Titanium dioxide (TiO₂), particularly in the anatase phase, is a favoured photoanode material due to its strong oxidation power, stability, cost-effectiveness, and non-toxicity [2]. However, the low electron mobility of $TiO₂$ limits its performance in DSSCs, making it imperative to explore methods to enhance its efficiency [3].

Previous studies have demonstrated that doping TiO2 with various materials can significantly enhance its electron mobility and overall DSSC efficiency. For instance, doping with materials such as copper (Cu), sulfur (S), and copper sulfide (CuS) has shown promising results. CuS, in particular, has been identified as a suitable dopant due to its appropriate particle size, high surface area, significant band gap reduction, and high Jsc values [4, 5].

Despite these advancements, there is a need for systematic research to optimize the doping concentration, photoanode thickness, and operating temperature to achieve maximum efficiency in DSSCs. This study aims to address these gaps by investigating the effects of doping TiO₂ with CuS and varying internal parameters to enhance DSSC performance. The findings from this research are expected to contribute significantly to developing DSSCs as a sustainable and efficient alternative to conventional solar cells, thereby addressing the global energy crisis.

Therefore, research devoted to developing enhanced TiO₂-based DSSCs through doping and parameter optimization is highly relevant.

2. Literature review and problem statement

Dye-Sensitized Solar Cells (DSSCs) have gained substantial attention as a promising alternative to conventional silicon-based solar cells due to their cost-effectiveness, ease

of fabrication, and environmental friendliness [1]. Despite these advantages, enhancing the efficiency of DSSCs remains a significant challenge, primarily due to the limitations of the photoanode material, typically titanium dioxide $(TiO₂)$.

Several studies have focused on doping $TiO₂$ with various materials to improve its electron mobility and overall efficiency. For instance, one study synthesized Cu-Ag co-doped $TiO₂$ thin films and achieved a maximum efficiency of 2.46 %. It demonstrated that doping $TiO₂$ could effectively reduce the band gap and improve electrical conductivity, thereby enhancing DSSC performance [6]. Their findings demonstrated that doping $TiO₂$ could effectively reduce the band gap and improve electrical conductivity. However, the research also highlighted the cost and complexity of the doping process, which poses significant challenges for large-scale application. Another study explored S-doped TiO₂ nanofibers and reported a significant increase in DSSC efficiency from 1.54 % to 4.27 % compared to undoped $TiO₂$. This improvement was attributed to the enhanced photon-to-electron conversion efficiency and better dye adsorption capacity of the S-doped $TiO₂$ nanofibers [7]. This improvement was attributed to enhanced photon-to-electron conversion efficiency and better dye adsorption capacity. Despite these promising results, the method involved complex hydrothermal treatments, making it less practical for industrial-scale production.

However, despite these advancements, several unresolved issues persist. The primary challenge lies in achieving consistent and reproducible enhancements in DSSC efficiency through doping. The variability in results can be attributed to differences in doping concentrations, fabrication methods, and the physical properties of the dopants themselves. For example, while Cu-Ag co-doping has shown promise, the cost and scalability of this approach remain concerns [6]. Similarly, the S-doping method, although effective, involves complex hydrothermal treatments that may not be practical for large-scale applications [7].

The objective difficulties associated with these approaches include the fundamental limitations of doping efficiency, the stability of doped materials under operational conditions, and the high cost of certain dopants and fabrication techniques. These issues make it imperative to explore alternative doping strategies and optimize existing methods to make DSSCs more viable for commercial use.

One potential solution is to explore using readily available and cost-effective dopants such as copper sulfide (CuS). CuS has been identified as a promising dopant due to its suitable particle size, high surface area, significant band gap reduction, and high Jsc values. A study reported that CuS-doped TiO2 exhibited enhanced electron mobility and better structural properties, leading to improved DSSC performance [4]. This study presents CuS as a cost-effective and readily available dopant. However, it provided a viable alternative, their work did not address long-term stability and potential degradation of the doped materials under operational conditions.

Previous attempts to enhance DSSC performance through doping have yielded mixed results. For instance, one study investigated Cu-doped $TiO₂$ and achieved an efficiency of 5.26 %. However, the doping process involves costly and complex hydrothermal methods, which limit its practical application [8]. Their work demonstrated the potential of Cu doping in improving DSSC performance. Nevertheless, the complexity and cost of the hydrothermal doping process limit its practical application. Similarly, another study used Er-Yb co-doping and achieved an efficiency of 13.45 %, but the use of rare earth elements makes this approach expensive and unsustainable [9]. This study highlights the trade-off between achieving high efficiency and maintaining cost-effectiveness and scalability.

These unresolved issues and objective difficulties indicate that further research is needed. All this suggests that it is advisable to conduct a study on optimizing doping strategies for $TiO₂$ in DSSCs, focusing on cost-effective, scalable, and efficient methods that can enhance electron mobility and overall device performance.

3. The aim and objectives of the study

The aim of the study is to optimize the efficiency of Dye-Sensitized Solar Cells (DSSCs) by enhancing the performance of $TiO₂$ photoanodes through targeted doping and the variation of internal parameters. This will enable the development of more efficient and sustainable DSSCs, contributing to the advancement of alternative energy solutions.

To achieve this aim, the following objectives are established: – systematically analyze the effects of different dopants (sulfur, copper, and copper sulfide) on the performance of $TiO₂$ -

based DSSCs; – compare the impact of each dopant on the efficiency of $TiO₂$ photoanodes, leveraging previous research findings;

– optimize the photoanode thickness by conducting experiments to identify the thickness that maximizes efficiency;

– assess the influence of various internal parameters, such as dopant concentration and temperature, on $TiO₂$ photoanode efficiency, and identify optimal conditions;

– investigate the combined effects of doping and internal parameter variations to enhance DSSC performance and identify synergistic interactions.

4. Materials and methods

The object of this research is Dye-Sensitized Solar Cells (DSSCs), specifically focusing on the performance enhancement of TiO₂-based photoanodes through doping and internal parameter variations.

Hypothesis of the study: doping $TiO₂$ photoanodes with elements like sulfur, copper, and copper sulfide, combined with optimization of internal parameters (e.g., concentration, thickness, and temperature), will significantly enhance the efficiency of DSSCs.

Assumptions made in the work:

1. The dopants uniformly integrate into the $TiO₂$ matrix without causing significant structural defects.

2. The simulation environment accurately replicates experimental conditions.

3. The interactions between dopants and $TiO₂$ are consistent across different conditions.

Simplifications adopted in the work:

1. The study assumes ideal conditions for dopant distribution and does not account for potential manufacturing inconsistencies.

2. Effects of external environmental factors such as humidity and light intensity variations are not considered.

3. The electron mobility and recombination rates are assumed to be consistent across all simulations.

This study utilized simulations to enhance DSSC performance, focusing on TiO₂-based photoanodes. Initial simulations replicated previous studies to validate internal parameters (Table 1). The resulting data, including current density and voltage (J-V) curves, provided a basis for analyzing the impact of variations in dopant concentration, photoanode thickness, and operational temperature on DSSC efficiency.

Internal parameters

The study employed several equations to simulate DSSC performance:

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

This equation calculates the current density, *J*, as a function of electron charge (*q*), *n* is the electron concentration, \upmu is the electron mobility, and E is the electric field.

Voltage:

$$
V_{OC} = \frac{kTm}{q} \ln \left[\left(\frac{LJ_{SC}}{qDn_0 \tanh\left(\frac{d}{L}\right)} \right) + 1 \right],\tag{2}
$$

where *V* is the voltage, *J* is the current density, and *R* is the resistance.

Efficiency (η):

$$
\eta = \frac{V_{oc}J_{sc}FF}{P_{in}} \times 100\%,\tag{3}
$$

where *Pout* is the output power, and *Pin* is the input power. Fill factor (*FF*):

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

where
$$
V_{mp}
$$
 is the maximum power point voltage, J_{mp} is the maximum power point current density, V_{oc} is the open-circuit voltage, and J_{sc} is the short-circuit current density.

Electron diffusion coefficient (*D*):

Table 1

$$
D = \frac{kT\mu}{q},\tag{5}
$$

where *D* is the electron diffusion coefficient; μ is the electron mobility; *k* is the Boltzmann's constant; T is the temperature; q is the electron charge.

The simulations were conducted using MATLAB software. MATLAB was used to code the mathematical models and solve the equations to model the physical processes within the DSSCs.

The simulations were set up under standard conditions with the internal parameters defined in Table 1. The temperature was maintained at 300 K and the light intensity was set to 1⋅10¹⁷ cm⁻²s⁻¹. Variations in the concentration of dopants, photoanode thickness, and temperature were systematically applied to analyze their effects on DSSC performance.

The models were validated by replicating results from previous studies and comparing them with experimental data from the literature. The accuracy of the models was confirmed by matching simulated J-V curves with those from earlier works. This validation ensured the reliability of the models before applying variations to the internal parameters.

By understanding how these parameters influence DSSC performance, this study provides insights into the optimal design and operation of DSSCs, contributing to the development of more efficient solar cells.

5. Research results: internal parameter variation of TiO2/CuS photoanode

5. 1. TiO2 undoped and doped replication

Table 2 shows the results of revising the J-V curves for pure and doped $TiO₂$ on DSSC photoanodes.

Fig. 1 illustrates the J-V curves for pure and doped $TiO₂$ on DSSC photoanodes.

Table 3 shows the results of the data replication for TiO₂ doping on DSSC photoanodes.

The data indicates that doping $TiO₂$ with CuS significantly enhances the efficiency of DSSCs compared to undoped TiO2. This improvement is attributed to the doped photoanode's enhanced electron mobility and better structural properties.

Table 2

Results data replication $TiO₂$ simulation was pure on DSSC photoanode

Material	$J_{\rm sc}$ (mA/cm ²)	$V_{oc}(V)$	$P_{\text{max}}\left(\text{mA/cm}^2\text{-V}\right)$	Eff (%) FF		References
TiO ₂ pure	15.38	0.71	6.53	0.60	6.53	This research
$TiO2$ pure	12.05	0.75	6.72	0.74	6.72	$[13]$
TiO ₂ pure	13.90	0.71	6.41	0.64	6.41	[5]
TiO ₂ pure	14.85	0.71	6.37	0.61	6.37	[4]

Fig. 1. Replication phenomenon physical J-V curve: $a - TiO₂$ pure; $b - TiO₂$ doped on DSSC photoanode

Results data replication simulation of $TiO₂$ doping on DSSC photoanode

Table 3

Table 4

5. 2. Variation of TiO2/CuS concentration

Table 4 presents the simulation results of $TiO₂/CuS$ concentration variations in the DSSC photoanode. Fig. 2 shows the corresponding J-V curves.

The optimal TiO₂/CuS doping concentration is 0.3%, achieving the highest efficiency. Concentrations higher than this result in diminished performance, likely due to increased recombination rates.

Simulation results of $TiO₂/CuS$ concentration variations in the DSSC photoanode

Concentration $(\%)$	$J_{\rm sc}$ (mA/cm ²)	$V_{oc}(V)$	$P_{\text{max}}\left(\text{mA}/\text{cm}^2\text{V}\right)$	FF	$Eff(\%)$
0.1%	14.72	0.71	7.55	0.72	7.55
0.2%	15.50	0.71	7.99	0.72	7.99
0.3%	15.84	0.71	8.18	0.73	8.18
0.4%	15.75	0.71	8.13	0.73	8.13
0.5%	15.59	0.71	8.04	0.72	8.04
0.6%	15.24	0.71	7.84	0.72	7.84
0.7%	14.54	0.71	7.44	0.72	7.44
0.8%	13.68	0.70	6.96	0.72	6.96
0.9%	11.27	0.69	5.61	0.72	5.61
1%	6.21	0.66	2.89	0.71	2.89

Table 5

Fig. 2. Variation concentration J-V curve of $TiO₂/CuS$ on DSSC photoanode

5. 3. Variation of TiO₂ thickness photoanode

Table 5 presents the simulation results data for various thicknesses of $TiO₂/CuS$ in the DSSC photoanode. Fig. 3 shows the corresponding J-V curves.

The optimal thickness for the $TiO₂/$ CuS photoanode is 3 μm, providing the best balance between light absorption and electron transport. Thicknesses greater than 3 μm lead to increased recombination, reducing efficiency.

5. 4. Variation of temperature

Table 6 presents the simulation results for temperature variations at the optimum thickness of $TiO₂/CuS$ on DSSC photoanodes. Fig. 4 illustrates the connection between thickness variation and efficiency at room temperature.

Higher temperatures enhance DSSC efficiency by improving electron mobility and reducing recombination rates. Optimal performance is observed at 325 K, suggesting temperature control is crucial for maximizing DSSC efficiency.

5. 5. Effect of combined internal parameter

Fig. 5 illustrates all the internal parameter combinations, which are concentration and thickness, of $TiO₂/CuS$ photoanode at every temperature (275 K, 300 K, 325 K), respectively.

Simulation results data for various thicknesses of $TiO₂/CuS$ in the DSSC photoanode

$d \text{(\mu m)}$	$J_{\rm sc}$ (mA/cm ²)	$V_{oc}(V)$	$P_{\text{max}}\left(\text{mA}/\text{cm}^2\text{-V}\right)$	FF	$Eff(\%)$
1	10.68	0.78	6.22	0.74	6.22
3	15.37	0.74	8.33	0.73	8.33
5	15.84	0.71	8.18	0.73	8.18
10	15.77	0.67	7.59	0.71	7.59
30	15.48	0.63	6.82	0.70	6.82
50	15.41	0.62	6.70	0.70	6.70
80	15.40	0.62	6.67	0.70	6.67
85	15.39	0.62	6.67	0.70	6.67
90	15.39	0.62	6.67	0.70	6.67
100	15.39	0.62	6.67	0.70	6.67

Fig. 3. Variation thickness J-V curve of $TiO₂/CuS$ on DSSC photoanode

Table 6

Results data simulation variation temperature at the optimum thickness of TiO₂/CuS on DSSC photoanode

Temperature (K)	$d \text{(\mu m)}$	J_{sc} (mA/cm ²)	$V_{oc}(V)$	$P_{\text{max}}\left(\text{mA/cm}^2\text{-V}\right)$	FF	Eff $(\%)$
275		15.37	1.25	13.94	0.72	13.94
300		15.37	1.36	15.06	0.72	15.06
325		15.37	1.46	16.18	0.72	16.18

Fig. 5. Internal parameter combination J-V curve of $TiO₂/CuS$ on DSSC photoanode at: *a –* 275 K; *b –* 300 K; *c –* 325 K

Higher temperatures enhance DSSC efficiency by improving voltage values. It means higher temperatures improve electricity energy production in supporting DSSC performance.

6. Discussion of results: internal parameter variation of TiO2/CuS photoanode

This study presents an in-depth analysis of the internal parameter variations in $TiO₂/CuS$ photoanodes, demonstrating significant performance improvements in dye-sensitized solar cells (DSSCs) through CuS doping.

The J-V curves shown in Fig. 1, *a*, *b* illustrate the comparison between pure and CuS -doped $TiO₂$ photoanodes. Both materials exhibit similar open-circuit voltage (*Voc*) values of approximately 0.7 V. However, the CuS-doped TiO2 photoanode significantly increases short-circuit current density (J_{sc}) . This increase is attributed to enhanced electron mobility facilitated by CuS doping. The improved

electron mobility leads to a higher diffusion coefficient (*D*), consistent with trends reported in previous studies [14]. Data obtained from Table 3 support this, showing that the CuS-doped $TiO₂$ photoanode achieves the highest efficiency and maximum power output (P_{max}) . This highlights the critical role of CuS in improving electron transport and photon absorption efficiency [15]. Thus, these results indicate that CuS doping can substantially enhance $J_{\rm sc}$ and the overall efficiency of DSSC devices.

The impact of varying CuS concentrations on DSSC performance is detailed in Table 4. The concentration variation from 0.1 % to 1 % shows that the optimal doping level is 0.3 %. At this concentration, the device achieves the highest efficiency of 8.18 %. Concentrations exceeding this point result in performance degradation, likely due to increased electron recombination rates. The J-V curves in Fig. 2 confirm that moderate CuS doping optimizes charge transport, enhancing overall device efficiency. In contrast, excessively high concentrations introduce defects that adversely affect device performance. These findings align with previous research, which also identified an optimal dopant concentration to maximize DSSC performance [4, 16].

The thickness of the $TiO₂/CuS$ photoanode plays a crucial role in DSSC performance, as shown in Table 5. The optimal thickness is identified as $3 \mu m$, which results in an efficiency of 8.33 %. The J-V curves in Fig. 3 indicate that increasing the photoanode thickness beyond this optimal point leads to a decline in efficiency due to increased recombination rates despite the higher potential for light absorption. These results emphasize the importance of balancing light absorption and electron transport in DSSC design. The efficiency improvement at this thickness is consistent with findings from other studies, which also emphasize the need for photoanode thickness optimization to achieve the best balance between photon absorption and charge transport [5, 15].

Temperature variations significantly impact DSSC efficiency, as shown in Table 6. Efficiency increases with temperature, peaking at 16.18 % at 325 K. This increase is attributed to enhanced electron mobility and reduced recombination rates at higher temperatures, as observed in the J-V curves in Fig. 4. This study highlights the importance of temperature control in maximizing DSSC performance. These findings are consistent with previous research, which also observed temperature-dependent efficiency trends [13, 16].

Fig. 5 presents the combined effects of CuS concentration, photoanode thickness, and temperature on DSSC performance. The optimal combination 0.3 % CuS doping, 3 μm photoanode thickness, and an operating temperature of 325 K yields the highest efficiency. These results underscore the synergistic interaction between these parameters, which is crucial for optimizing DSSC performance. The findings are consistent with the literature highlighting the necessity of fine-tuning multiple internal parameters to achieve optimal solar cell efficiency [16].

However, despite these promising results, there are challenges related to the scalability and cost implications of the CuS doping process. Additionally, while the current study provides substantial evidence supporting the efficacy of CuS doping, further experimental validation is necessary to confirm these findings under varying conditions. Variability in experimental setups can lead to discrepancies in reproducibility, emphasizing the need for rigorous validation.

7. Conclusions

1. Doping TiO2 with CuS significantly enhances electron mobility, leading to an 8.18 % increase in efficiency. This demonstrates the effectiveness of CuS doping in improving DSSC performance by boosting current density (*Jsc*).

2. CuS doping was found to outperform both Cu and S dopants. The $TiO₂/CuS$ photoanode achieved higher efficiencies, specifically improving the structural and electronic properties of the photoanode. This superior performance underscores the potential of CuS as a more effective dopant, with a maximum efficiency improvement of 16.18 % observed under optimal conditions.

3. The study determined that a photoanode thickness of 3 μm is optimal, achieving an efficiency of 8.33 %. This thickness offers the best balance between photon absorption and electron transport, enhancing overall DSSC performance.

4. The highest efficiency of 8.18 % was achieved at a CuS concentration of 0.3 %, optimizing the balance between conductivity and recombination. Temperature variations also significantly influenced DSSC performance, with efficiency values increasing to 13.94 %, 15.06 %, and 16.18 % at temperatures of 275 K, 300 K, and 325 K, respectively.

5. The study identified synergies between CuS doping and internal parameter optimization, particularly temperature. Higher temperatures improved electron mobility and diffusion coefficients, leading to substantial efficiency gains.

Conflict of interest

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

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Data availability

Data will be made available at a reasonable request.

Use of artificial intelligence

The authors have used artificial intelligence technologies within acceptable limits to provide their own verified data, which is described in the research methodology section.

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