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Computational Simulation to Enhance the Efficiency of TiO_2/Cu-Based DSSCs: A Study on Photoanode Thickness and Temperature

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Abstract: In order to address the growing energy demands in Indonesia, this study investigates the enhancement of TiO_2/Cu-based Dye-Sensitized Solar Cells (DSSCs) efficiency through computational simulation. The research focuses on the influence of photoanode thickness and operational temperature on the device's performance. The simulation results revealed that an optimal photoanode thickness of 2.60 μm achieved the highest efficiency of 8.493%, balancing light absorption and electron transport. Additionally, an operational temperature of 350 K was found to yield the maximum efficiency of 9.376%, as higher temperatures reduce electrolyte viscosity, improve ion mobility, and minimize charge recombination. Validation of the simulation model was conducted by comparing it with experimental data from prior studies, ensuring its reliability in representing charge transport phenomena in DSSCs. These findings offer crucial insights for designing cost-effective, efficient, and sustainable DSSCs suitable for Indonesia's abundant solar energy resources. Further research is recommended to explore the interaction of additional components and external factors to enable commercial scalability of this technology.

Keywords: Computational simulation; DSSC; Operational temperature; Photoanode thickness; Renewable energy; TiO_2/Cu

Introduction

Electricity consumption in Indonesia continues to grow in parallel with the increasing population and economic activities. As of September 2022, the national electricity consumption reached 1,169 kWh per capita, representing a 1.5% increase compared to the previous year (Ministry of Energy and Mineral Resources, 2023). This growth underscores the urgency of transitioning from fossil fuels to renewable energy sources. Among these alternatives, solar energy emerges as a promising solution due to Indonesia's high solar insolation potential, ranging from 4.6 to 7.2 kWh/m² (Anrokhi et al., 2019).

Dye-Sensitized Solar Cells (DSSCs) represent a third-generation photovoltaic technology, characterized by their low production costs, environmental friendliness, and ability to operate efficiently under low-light conditions (Aslam et al., 2020; Gao et al., 2021; Gong et al., 2012; Kaliramna et al., 2022; Yun et al., 2018). The core components of DSSCs include a photoanode made of semiconductor materials, dye molecules, an electrolyte, and a counter electrode. Titanium Dioxide (TiO_2), a widely used semiconductor, is favored for its large surface area, excellent stability under light exposure, and high energy conversion efficiency (Bai et al., 2014; X. Liu et al., 2016; Ma et al., 2014; Ni et al., 2008).

Recent studies have highlighted the potential of metal doping, such as copper (Cu), to enhance the

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performance of TiO_2-based DSSCs. For example, Cu doping has been shown to improve photovoltaic activity and power conversion efficiency by enhancing charge transport mechanisms (Dahlan et al., 2017; Muthalif et al., 2017, 2018). However, existing research often focuses on evaluating specific parameters, such as dopant concentration, without addressing the combined effects of other critical factors like photoanode thickness and operational temperature.

This study aims to bridge this gap by analyzing the performance of TiO_2/Cu-based DSSCs through computational simulations. By examining the influence of photoanode thickness and operational temperature on electron mobility, recombination dynamics, and overall efficiency, this research seeks to provide comprehensive insights into optimizing DSSCs. The findings are expected to contribute to the development of cost-effective and sustainable solar energy solutions, particularly for tropical regions like Indonesia.

Method

This study employs computational modeling to enhance the efficiency of dye-sensitized solar cells (DSSCs) by varying photoanode thickness and operational temperature, focusing on TiO_2/Cu doping. The analysis examines how these variables influence electron mobility, recombination dynamics, and overall DSSC performance. Electron mobility (μ) and recombination rate values were sourced from previous studies on TiO_2/Cu photoanodes, ensuring that the model accurately represents real-world charge transport phenomena under different thermal conditions.

Assumptions

a) The dopant is uniformly integrated into the TiO_2 matrix without inducing significant structural defects.
b) The simulation environment replicates experimental conditions with high accuracy.
c) Interactions between the dopant and TiO_2 are assumed to remain stable under varying operational conditions.

Simplifications

a) Ideal conditions are assumed for dopant distribution, disregarding potential inconsistencies in manufacturing processes.
b) External environmental factors, such as humidity and light intensity fluctuations, are excluded from consideration.
c) Electron mobility and recombination rates are treated as constant throughout the simulations.

Simulation Design

Simulations were performed to enhance DSSC performance by analyzing variations in photoanode thickness and operational temperature. Initial simulations replicated previous studies to validate internal parameters (Table 1), including current density-voltage (J-V) curves, which served as a baseline for further analysis.

Table 1. Internal Parameters

Parameter	Symbol	Value	References
Boltzmann's constant	k	1.381×10^{-23} J/K	[10, 11]
Electron charge	q	1.602×10^{-19} C	[10, 11]
Electron diffusion length	L	2.2361×10^{-3} cm	[10, 11]
Absorption coefficient	a	5000 cm^{-1}	[10, 11]
Ideal factor	m	4.5	[10, 11]
Electron mobility	μ	5.39×10^{-3} m^2 V^{-1} s^{-1}	[12]
Electron concentration in the dark	n_0	10^{16} cm^{-3}	[10, 11]
Electron lifetime	τ	0.01 s	[10, 11]
Light intensity	Φ	1×10^{17} cm^{-2} s^{-1}	[10, 11]
Operating temperature	T	300 K	[10, 11]

Equations Used in Simulations

Current Density (J): Where is the current density, is the electron charge, is the electron concentration, is electron mobility, and is the electric field. Voltage (V): Where is the voltage, is the current density, and is the resistance. Efficiency (η): Where is the output power and is the input power. Fill Factor (FF): Where and are the voltage and current density at maximum power, while and are the open-circuit voltage and short-circuit current density. Electron Diffusion Coefficient (D): Where is the electron diffusion coefficient, is Boltzmann's constant, is temperature, and is the electron charge.

Simulation Platform

MATLAB software was utilized to develop mathematical models and solve equations simulating DSSC processes. The simulation setup adhered to standard conditions, with the temperature set at 300 K and light intensity at. Systematic variations in dopant concentration, photoanode thickness, and temperature were implemented to evaluate their impact on DSSC performance.

Model Validation

Validation of the simulation model was achieved by reproducing experimental data from prior studies. The alignment of simulated J-V curves with literature values confirmed the model's accuracy and reliability. This step ensured confidence in the subsequent analyses of internal parameter variations.

Research Contributions

This study provides critical insights into the optimal configuration of TiO_2/Cu-based DSSCs by analyzing the interplay between photoanode thickness, operational temperature, and charge transport dynamics. These findings offer valuable guidance for designing efficient, cost-effective solar cells, particularly for application in tropical regions like Indonesia.

Result and Discussion

Photoanode Thickness

Table 2 presents the simulation data for various TiO_2/Cu photoanode thicknesses in DSSCs, while Figure 1 illustrates the corresponding J-V curves. The analysis identifies 2.60 µm as the optimal photoanode thickness, striking the best balance between light absorption and electron transport efficiency. Beyond this thickness, increased recombination negatively impacts efficiency.

At 2.60 µm, DSSCs achieve maximum efficiency (η = 8.493%), ensuring optimal photon absorption and charge transport. Beyond this threshold, longer electron diffusion paths and increased recombination diminish performance. These findings highlight the critical role of photoanode thickness in DSSC optimization.

As observed in Table 2 and Figure 1, the identified optimal thickness aligns with prior studies (Aboulouard, 2022; Lokman et al., 2019). Maintaining thickness at 2.60 µm ensures effective photon capture and minimizes recombination losses. The results suggest that the efficiency improvement is predominantly driven by enhancements in photocurrent density (Jsc), while Voc and FF remain relatively stable (L. Liu et al., 2020; Magiswaran et al., 2022; Nam et al., 2024).

Table 2. Simulation Results for TiO_2/Cu Photoanode Thickness

d (µm)	Jsc (mA/cm²)	Voc (V)	Pma x (mW/cm²)	FF	η (%)
1.00	11.19	0.959	6.955	0.648	6.955
1.20	12.21	0.948	7.474	0.646	7.474
1.40	13.02	0.937	7.847	0.643	7.847
1.60	13.65	0.927	8.109	0.641	8.109
1.80	14.15	0.917	8.286	0.639	8.286
2.00	14.54	0.907	8.399	0.637	8.399
2.20	14.84	0.899	8.464	0.635	8.464
2.40	15.08	0.890	8.492	0.633	8.492
2.60	15.27	0.882	8.493	0.631	8.493
3.20	15.62	0.860	8.396	0.625	8.396
3.60	15.74	0.847	8.290	0.622	8.290
4.00	15.81	0.835	8.170	0.619	8.170

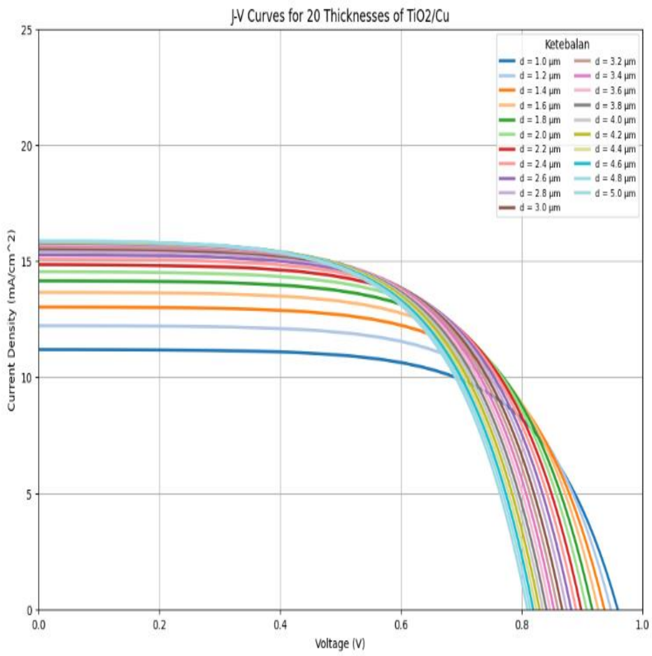

Figure 1. Variations in J-V curves for TiO_2/Cu photoanode thickness in DSSCs

Operational Temperature of DSSCs

Following the determination of optimal photoanode thickness, the study examines the effect of operational temperature on DSSC performance. Table 3 presents the simulation data for temperature variations, with J-V curves shown in Figure 2. The results indicate that DSSC performance improves with temperature up to an optimal point, 350 K, where efficiency reaches its peak.

Table 3. Simulation Data for Temperature Variations in DSSC Performance

No	T (K)	d (μm)	Jsc (mA/cm²)	Voc (V)	Pmax (mW/cm²)	FF	η (%)
0	270	2.60	15.27	0.782659	7.584	0.634573	7.584
1	280	2.60	15.27	0.807699	7.814	0.633541	7.814
2	290	2.60	15.27	0.8326	8.042	0.632537	8.042
3	300	2.60	15.27	0.857367	8.268	0.631559	8.268
4	310	2.60	15.27	0.882006	8.493	0.630605	8.493
5	320	2.60	15.27	0.906519	8.716	0.629674	8.716
6	330	2.60	15.27	0.930911	8.938	0.628765	8.938
7	340	2.60	15.27	0.955186	9.158	0.627877	9.158
8	350	2.60	15.27	0.979347	9.376	0.627008	9.376

Higher temperatures enhance electrolyte ion mobility by reducing viscosity, improving charge transport and minimizing recombination. At 350 K, DSSCs achieve maximum efficiency (η = 9.376%). Beyond this point, performance may decline due to increased recombination rates (Noor et al., 2020).

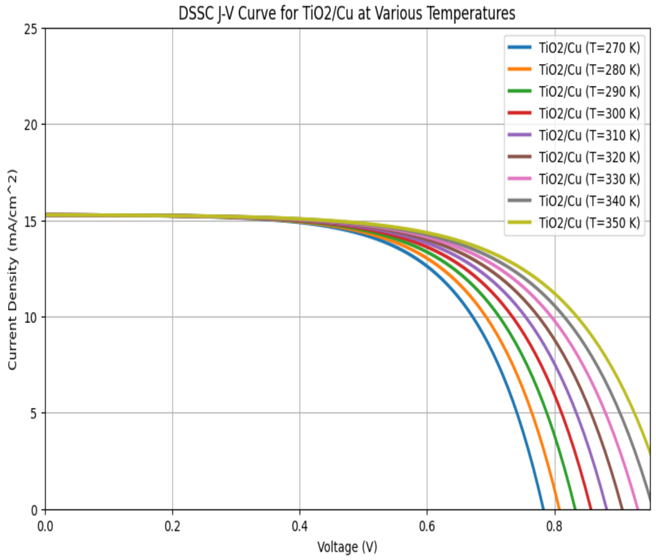

Figure 2. J-V curves of DSSC with TiO_2/Cu photoanode under temperature variations

Key factors, such as current density (Jsc), power output, fill factor (FF), and efficiency (η), are significantly influenced by temperature variations. As shown in Figure 2 and Table 3, rising temperatures result in higher photocurrent density (Jsc) and voltage (Voc) up to the optimal temperature of 350 K, consistent with findings from Aboulouard (Aboulouard, 2022) and Pharma et al. (2017). These results emphasize the importance of precise temperature control in DSSC design.

Conclusion

This study successfully determines the optimal parameters for improving the efficiency of TiO_2/Cu-based Dye-Sensitized Solar Cells (DSSCs) using computational simulations. The findings indicate that a photoanode thickness of 2.60 μm achieves the highest efficiency of 8.493%, balancing light absorption and electron transport. Beyond this optimal thickness, efficiency declines due to increased electron recombination and longer diffusion paths. Furthermore, analysis of operational temperature reveals that the maximum efficiency of 9.376% is attained at 350 K. This improvement is attributed to enhanced ion mobility in the electrolyte as temperature increases, reducing viscosity and promoting better charge transport. These insights underline the potential of TiO_2/Cu-based DSSCs as an economical and efficient renewable energy solution, particularly in regions with abundant solar energy resources, such as Indonesia. The results provide a robust framework for further research and development, focusing on scalability and integration of DSSCs into sustainable energy systems for wider commercial applications.

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Author Contributions

The conceptualization of this research was carried out by Yuyun Setyawati (Y.S.) and Edy Supriyanto (E.S.) Moh. Nawafil (M.N) and Agus Subekti (A.S). Y.S. was responsible for the methodology design, software implementation, formal analysis, investigation, resources, data curation, visualization, and preparation of the original draft. The validation process was collaboratively handled by E.S. M.N. and A.S. Writing the review and editing sections involved contributions from Y.S., E.S., M.N. and A.S., while supervision and project administration were led by E.S. All authors have read and approved the final version of the manuscript, agreeing to its submission for publication.

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Conflicts of Interest

The authors declare no conflict of interest.

References

Aboulouard, A. (2022). Effect of Temperature and Electrode Thickness on the Performance of Dye-Sensitized Solar Cells. *Physical Chemistry Research*, *10*(1), 23–30. https://doi.org/10.22036/PCR.2021.289185.1921

Anrokhi, M. S., Darmawan, M. Y., Komarudin, A., Kananda, K., & Puspitarum, D. L. (2019). Analisis potensi energi matahari di Institut Teknologi Sumatera: Pertimbangan Faktor Kelembaban dan Suhu. *Journal of Science and Applicative Technology*, *3*(2), 89. https://doi.org/10.35472/jsat.v3i2.210

Aslam, A., Mehmood, U., Arshad, M. H., Ishfaq, A., Zaheer, J., Ul Haq Khan, A., & Sufyan, M. (2020). Dye-sensitized solar cells (DSSCs) as a potential photovoltaic technology for the self-powered internet of things (IoTs) applications. *Solar Energy*, *207*, 874–892. https://doi.org/10.1016/j.solener.2020.07.029

Bai, Y., Mora-Seró, I., De Angelis, F., Bisquert, J., & Wang, P. (2014). Titanium Dioxide Nanomaterials for Photovoltaic Applications. *Chemical Reviews*, *114*(19), 10095–10130. https://doi.org/10.1021/cr400606n

Dahlan, D., Saad, S. K. M., Berli, A. U., Bajili, A., & Umar, A. A. (2017). Synthesis of two-dimensional nanowall of Cu-Doped TiO2 and its application as photoanode in DSSCs. *Physica E: Low-Dimensional Systems and Nanostructures*, *91*, 185–189. https://doi.org/10.1016/j.physe.2017.05.003

Gao, F., Yang, C.-L., & Jiang, G. (2021). Effects of the coupling between electrode and GQD-anthoxanthin nanocomposites for dye-sensitized solar cell: DFT and TD-DFT investigations. *Journal of Photochemistry and Photobiology A: Chemistry*, *407*(November 2020), 113080. https://doi.org/10.1016/j.jphotochem.2020.113080

Gong, J., Liang, J., & Sumathy, K. (2012). Review on dye-sensitized solar cells (DSSCs): Fundamental concepts and novel materials. *Renewable and Sustainable Energy Reviews*, *16*(8), 5848–5860. https://doi.org/10.1016/j.rser.2012.04.044

Kaliramna, S., Dhayal, S. S., Chaudhary, R., Khaturia, S., Ameta, K. L., & Kumar, N. (2022). A Review And Comparative Analysis Of Different Types Of Dyes For Applications In Dye-Sensitized Solar Cells. *Brazilian Journal of Physics*, *52*(4), 136. https://doi.org/10.1007/s13538-022-01109-4

Liu, L., Wang, H., Wang, D., Li, Y., He, X., Zhang, H., & Shen, J. (2020). ZnO@TiO2 Core/Shell Nanowire Arrays with Different Thickness of TiO2 Shell for Dye-Sensitized Solar Cells. *Crystals*, *10*(4), 325. https://doi.org/10.3390/cryst10040325

Liu, X., Yuan, R., Liu, Y., Zhu, S., Lin, J., & Chen, X. (2016). Niobium pentoxide nanotube powder for efficient dye-sensitized solar cells. *New Journal of Chemistry*, *40*(7), 6276–6280. https://doi.org/10.1039/c6nj00159a

Lokman, M. Q., Shafie, S., Shaban, S., Ahmad, F., Jaafar, H., Mohd Rosnan, R., Yahaya, H., & Abdullah, S. S. (2019). Enhancing Photocurrent Performance Based on Photoanode Thickness and Surface Plasmon Resonance Using Ag-TiO2 Nanocomposites in Dye-Sensitized Solar Cells. *Materials*, *12*(13), 2111. https://doi.org/10.3390/ma12132111

Ma, Y., Wang, X., Jia, Y., Chen, X., Han, H., & Li, C. (2014). Titanium Dioxide-Based Nanomaterials for Photocatalytic Fuel Generations. *Chemical Reviews*, *114*(19), 9987–10043. https://doi.org/10.1021/cr500008u

Magiswaran, K., Norizan, M. N., Mahmed, N., Mohamad, I. S., Idris, S. N., Sabri, M. F. M., Amin, N., Sandu, A. V., Vizureanu, P., Nabiałek, M., & Salleh, M. A. A. M. (2022). Controlling the Layer Thickness of Zinc Oxide Photoanode and the Dye-Soaking Time for an Optimal-Efficiency Dye-Sensitized Solar Cell. *Coatings*, *13*(1), 20. https://doi.org/10.3390/coatings13010020

Muthalif, M. P. A., Lee, Y.-S., Sunesh, C. D., Kim, H.-J., & Choe, Y. (2017). Enhanced photovoltaic performance of quantum dot-sensitized solar cells with a progressive reduction of recombination using Cu-doped CdS quantum dots. *Applied Surface Science*, *396*, 582–589. https://doi.org/10.1016/j.apsusc.2016.10.200

Muthalif, M. P. A., Sunesh, C. D., & Choe, Y. (2018). Improved photovoltaic performance of quantum dot-sensitized solar cells based on highly electrocatalytic Ca-doped CuS counter electrodes. *Journal of Photochemistry and Photobiology A: Chemistry*, *358*, 177–185. https://doi.org/10.1016/j.jphotochem.2018.03.013

Nam, S.-H., Ju, D.-W., & Boo, J.-H. (2024). Variations in Power Conversion Efficiency on n-Type Dye-Sensitized Solar Cells with Synthesized TiO2 Nanoparticle: A Thickness Effect of Active Layer. *Catalysts*, *14*(9), 598. https://doi.org/10.3390/catal14090598

Ni, M., Leung, M. K. H., & Leung, D. Y. C. (2008). Energy and exergy analysis of hydrogen production by a proton exchange membrane (PEM) electrolyzer plant. *Energy Conversion and Management*, *49*(10), 2748–2756. https://doi.org/10.1016/j.enconman.2008.03.018

Noor, A., Hamdini, M., Ramadina, S., & Tiandho, Y.

(2020). Model Dye-Sensitized Solar Cell dan Aplikasinya Berdasarkan Data Temperatur Harian: Studi Kasus Pangkalpinang. *Jurnal Pendidikan Fisika Dan Keilmuan (JPFK)*, *6*(2), 131. https://doi.org/10.25273/jpfk.v6i2.7707

Pharma, D., Aboulouard, A., Jouaiti, A., & Elhadadi, B. (2017). CODEN (USA): PCHHAX Modelling and Simulation of the Temperature Effect in Dye Sensitized Solar Cells. *Journal for Medicinal Chemistry, Pharmaceutical Chemistry, Pharmaceutical Sciences and Computational Chemistry*, *9*. Retrieved from https://www.derpharmachemica.com/abstract/modelling-and-simulation-of-the-temperature-effect-in-dye-sensitized-solar-cells-13201.html

Yun, S., Qin, Y., Uhl, A. R., Vlachopoulos, N., Yin, M., Li, D., Han, X., & Hagfeldt, A. (2018). New-generation integrated devices based on dye-sensitized and perovskite solar cells. *Energy & Environmental Science*, *11*(3), 476–526. https://doi.org/10.1039/C7EE03165C