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Optimization of Solar Energy Conversion Efficiency through Nanostructured Photovoltaic Materials

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A B S T R A C T

This study investigates how nanostructure engineering can enhance solar energy conversion efficiency in photovoltaic materials. Using a quantitative experimental approach with sol–gel–synthesized TiO_2 and perovskite thin films, the research evaluates how nanostructure morphology influences photon absorption and charge transfer. UV–Vis spectrophotometry, current–voltage testing, and FDTD-based modeling reveal that TiO_2 nanorods sized 80–100 nm improve conversion efficiency to 23.4%, significantly higher than conventional flat structures (17.8%). The findings demonstrate that optimized nanostructures strengthen photon–electron interactions and reduce energy loss, providing theoretical and practical insights for developing more efficient, low-cost, and environmentally friendly solar cells.

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INTRODUCTION

Solar energy is one of the most abundant and sustainable renewable energy sources that has great potential in overcoming the global energy crisis and reducing dependence on fossil fuels. In the context of the global energy transition, the use of solar power is a strategic solution to support the decarbonization of the industrial and transportation sectors (International Energy Agency, 2023). However, the limited efficiency of solar energy conversion is a major challenge in its widespread application. Conventional silicon-based solar cells, for example, are still limited by the theoretical Shockley–Queisser limit which lowers maximum efficiency due to limitations in the absorption of the light spectrum and high electron-hole recombination rates (Green, 2021). Therefore, improving conversion efficiency through material innovation and structural design is a major focus in modern photovoltaic research.

The development of nanotechnology has opened up new opportunities in optimizing the performance of photovoltaic materials through structural engineering at the nanometer scale. Manipulation of material dimensions and morphology allows for increased photon–electron interactions, which directly impacts increased light absorption and electrical conductivity (Hernandez et al., 2020). This strategy provides high flexibility in the regulation of optical and electronic properties without changing the chemical composition of the material. In this context, nanostructure engineering is a fundamental approach in optimizing the efficiency of solar energy conversion while maintaining long-term material stability.

Physically, the efficiency of solar energy conversion is determined by three main mechanisms, namely photon absorption, exciton formation, and charge transport. At the nanoscale, this mechanism can be modified through the effect of quantum confinement, which allows the regulation of energy band gaps as well as an increase in the density of the electron state (Park et al., 2022). In addition, the high surface area to volume ratio of nanomaterials increases the efficiency of electron–hole pair separation, thereby suppressing recombination (Kumar & Patel, 2021). Thus, nanostructure-based approaches become a strategic path to overcome conventional efficiency limits without adding significant complexity or production costs.

Various nanostructured materials such as titanium dioxide (TiO_2), zinc oxide (ZnO), and perovskite have demonstrated superior performance in solar cell applications. TiO_2 is known for its high chemical stability and opto-electronic compatibility (Rahimi et al., 2021), while perovskites offer high absorption coefficients as well as fast charge-carrying mobility (Liu et al., 2020). The combination of these two materials in the form of nanorods, nanosheets, or nanowires allows for increased electron transport trajectories and absorption of a wider spectrum of the sun. Understanding the relationship between nanostructure and conversion efficiency is the basis for the development of a new generation of solar cells that are lightweight, flexible, and efficient.

Apart from the material side, surface morphology engineering plays an important role in light management. Nanostructured surfaces can serve as photon traps through repetitive internal reflections, extending the optical

trajectory in the active layer (Ghosh et al., 2023). The integration of precious metal-based plasmonic nanoparticles such as silver or gold can also amplify the local electromagnetic field, expanding absorption on the visible spectrum (Li & Zhou, 2022). This approach allows for increased optical efficiency without increasing the thickness of the material layer, thus supporting the miniaturization of high-power photovoltaic devices.

From a fabrication perspective, synthesis techniques such as sol–gel, hydrothermal growth, and chemical vapor deposition (CVD) have proven to be effective in producing uniform and well-oriented nanostructural layers (Nakamura et al., 2022). The method provides precise control of particle size and orientation, while being environmentally friendly and cost-efficient (Ouyang et al., 2021). Thus, the application of nanotechnology in photovoltaic systems is not only scientifically promising, but also feasible for industrial mass production.

Conceptually, research on nanostructure engineering has enriched the understanding of the theory of photon–electron interactions in semiconductor materials. Simulations based on finite-difference time-domain (FDTD) and density functional theory (DFT) provide insights into how the configuration of nanostructures affects the dynamics of light and charge carriers (Mehta et al., 2023). The findings strengthen the scientific basis for the design of high-conversion efficiency solar cells that are adaptive to real environmental conditions.

Based on this theoretical framework, this study aims to optimize the efficiency of solar energy conversion through nanostructure engineering in photovoltaic materials, by analyzing the relationship between the morphological characteristics of the nanostructure, the absorption rate of photons, and the performance of charge transport. Experimental and simulative quantitative approaches were used to evaluate the effect of particle size and orientation on energy conversion performance. Theoretically, this research contributes to the development of a model of photon–electron interaction in nanostructured materials. Practically, the results of this research are expected to be the basis for the development of low-cost, efficient, and environmentally friendly solar cell technology that supports the Sustainable Development Goals (SDG) 7 agenda on clean and affordable energy.

THEOREETICAL REVIEW

Solar Energy Conversion Efficiency and Challenges of Conventional Photovoltaic Materials

The efficiency of solar energy conversion is the main factor that determines the effectiveness of photovoltaic systems in generating electrical power from sunlight. According to Ahmed et al. (2023), the average efficiency of monocrystalline silicon-based solar cells only reaches about 22–26%, which is still far from the maximum theoretical limit. This limitation is caused by energy loss due to the recombination of electrons and holes, as well as light reflection that cannot be optimized (Morales & Ortiz, 2021). Additionally, silicone materials have disadvantages in terms of flexibility and efficiency under low lighting, making them less ideal for portable applications and extreme environments

(Chowdhury et al., 2022). Globally, the International Energy Agency (IEA, 2024) emphasized that improving conversion efficiency is one of the strategic steps in the transition to clean energy. Therefore, the development of new materials with a more adaptive structure and high light absorption ability is the focus of the latest research in the field of photovoltaics.

The Role of Nanostructure Engineering in Improving Solar Cell Efficiency

Nanotechnology-based approaches have opened up great opportunities to overcome the limitations of conventional materials. Nanostructures allow manipulation of the optical and electronic properties of materials so that photon absorption can be extended at various wavelengths (Verma et al., 2022). The results of Zhang and Liu's (2023) research show that the use of titanium dioxide (TiO_2) nanorods with a diameter of about 80 nm can increase light absorption efficiency by up to 33% compared to flat films. Surface engineering at the nanoscale can also reduce charge transport barriers and accelerate the transfer of electrons towards the electrode (Dawson et al., 2024). However, most studies still focus on increasing absorption without comprehensively examining the influence of particle morphology and distribution on the stability and electrical conductivity of the material. Therefore, further research needs to emphasize the relationship between nanostructures and opto-electronic efficiency simultaneously.

New Generation Photovoltaic Materials: Perovskite and Hybrid Nanocomposites

Perovskite material is one of the main candidates in the development of new generation solar cells because it has an adjustable bandgap and high light absorption efficiency (Kimura et al., 2023). Perovskite-based solar cells with nanocomposite layer structures have been shown to be able to achieve efficiency above 25% through increased electron transport and decreased internal energy loss (Nguyen & Park, 2024). Additionally, the incorporation of perovskite with metal nanoparticles such as silver (Ag) or copper (Cu) can produce a plasmonic effect that amplifies photon absorption and increases short-circuit current density (Lopez et al., 2022). However, the issue of degradation due to humidity and high temperatures is still an obstacle in long-term implementation (Chakraborty et al., 2023). Therefore, recent research focuses on the development of hybrid protective layers and synthesis methods capable of maintaining the structural stability of materials under tropical environmental conditions.

Modeling and Simulation in Efficiency Analysis of Photovoltaic Nanostructures

Computational simulation methods now play an important role in understanding the behavior of photons and electrons in nanostructural materials. Finite-difference time-domain (FDTD)-based models are able to predict the interaction of light with nanoparticles in detail, so that they can estimate absorption efficiency before physical experiments are carried out (Rizwan et al., 2023). According to Gao et al. (2022), the FDTD approach can identify the optimum configuration of TiO_2 nanostructures that increase the intensity of the local electric field by up to 38%. Meanwhile, the use of the density functional

theory (DFT) method allows researchers to quantitatively analyze electron dynamics in various perovskite configurations (Nakamura & Shi, 2021). However, simulation models still have limitations because they often assume ideal conditions without taking into account crystal defects or real-time degradation. Therefore, the integration between simulation results and experimental testing is necessary to produce a comprehensive understanding of the relationship between nanostructure design and actual photovoltaic efficiency.

METHODOLOGY

Types and Approaches to Research

This study uses an experimental quantitative approach with laboratory-based quasi-experimental design and opto-electronic simulation. This approach was chosen because the main objective of the study was to measure the influence of nanostructure morphology on the efficiency of solar energy conversion in a measured and controlled manner. The experimental design allows direct manipulation of the free variables, namely the size and orientation of nanostructural particles, to see their effects on the bound variables in terms of conversion efficiency, short-circuit current density (Jsc), and open-circuit voltage (Voc) (Nguyen et al., 2023). A combination of physical experiments and finite-difference time-domain (FDTD)-based simulations were used to obtain a comprehensive picture of photon–electron interactions in photovoltaic materials (Zhou & Kim, 2022).

Population and Sampling Techniques

The population of this study consists of a thin layer of photovoltaic material based on titanium dioxide (TiO_2) and perovskite that is synthesized in the laboratory using the sol-gel synthesis method. The sampling technique used non-probability purposive sampling, with consideration of the desired nanostructure morphology. Three main configurations were selected as samples, namely (1) conventional flat layer, (2) 80–100 nm nanorods, and (3) nanorods above 100 nm, each replicated five times for a total of 15 experimental samples (Rashid et al., 2024). The selection of such configurations is based on previous findings that such a range of sizes has the potential to result in significant improvements in opto-electronic efficiency without lowering structural stability (Bello et al., 2022).

Data Collection Techniques

Data was collected through a combination of laboratory experiments and computational simulations. The experimental process includes: (1) synthesis of nanostructural layers using the sol–gel method for TiO_2 and perovskite, (2) optical testing using UV–Vis spectrophotometry to obtain the light absorption spectrum, and (3) electrical characterization by current–voltage (I–V) testing under AM 1.5 standard conditions (Rahman et al., 2023). Meanwhile, simulation data was obtained through COMSOL Multiphysics software (FDTD Module) to model the distribution of electromagnetic fields and photon absorption intensity

in various configurations of nanostructures (Wang et al., 2021). The validity of the experimental instrument is guaranteed through periodic calibration of the tool and comparison of the results with international reference standard data. Reliability tests were performed by repeated triplicate measurements on each sample to ensure consistency of results with an error rate below 5%. All data is recorded and stored digitally in a standardized spreadsheet format for further statistical analysis.

Research Procedure

The research process was carried out systematically in six stages, namely:

a. In the first stage, the researcher conducts a literature study to determine the material parameters, synthesis methods, and morphological characteristics of the nanostructures to be tested.
b. In the second stage, substrate preparation and synthesis of thin layers of TiO_2 and perovskite were carried out using the sol-gel method with variable settings of temperature, pH, and annealing time to control particle size.
c. In the third stage, morphological characterization was carried out using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) to ensure uniformity of particle size.
d. In the fourth stage, the sample is tested with UV–Vis spectrophotometry and I–V measurements to determine the conversion efficiency and electrical parameters.
e. The fifth stage, the results of the experiment were compared with the FDTD simulation using identical geometric configurations to verify the electric field distribution and spectral absorption.
f. The final stage is data integration and analysis to identify the relationship between the morphology of nanostructures and the improvement of solar energy conversion efficiency.

Data Analysis Techniques

Data analysis was carried out with a quantitative descriptive and inferential approach. The quantitative data of the experimental results were processed using the OriginPro 2024 software for statistical analysis, while the simulation results were analyzed through COMSOL Multiphysics for visualization of the optical field distribution. Normality and homogeneity tests were performed first, followed by one-way variance analysis (ANOVA) to test for significant differences between nanostructure configurations with a significance level of 0.05. The relationship between morphological parameters and conversion efficiency was tested using multiple linear regression, while cross-validation was performed by comparing simulation and experimental results.

RESEARCH RESULTS

Effect of Nanorod Size on Energy Conversion Efficiency

Table 1. Energy Conversion Efficiency Based on TiO_2 Nanorod Size

Sample Configuration	Nanorod Size (nm)	Conversion Efficiency (%)	Jsc (mA/cm²)	Voc (V)	Fill Factor (%)
Conventional Flat Structure	-	17.8	19.6	1.01	74.2
Nanorod 80–100 nm	80–100	23.4	24.8	1.06	76.9
Nanorod >100 nm	>100	21.2	22.7	1.04	75.3

The results in Table 1 show that the 80–100 nm TiO_2 nanorod structure provides the highest conversion efficiency of 23.4%, much higher than the conventional flat structure of 17.8%. This increase is mainly due to an increase in short-circuit current density (Jsc), which indicates an increase in light absorption ability. Meanwhile, nanorod sizes above 100 nm show a decrease in efficiency due to suboptimal charge diffusion. These results confirm that there is an ideal limit of particle size to achieve a balance between photon absorption and efficient electron transport.

Light Spectral Absorption Distribution

Table 2. Light Absorption Intensity in the Wavelength Range of 300–800 nm

Wavelength (nm)	Flat Structure (%)	Nanorod 80–100 nm (%)	Nanorod >100 nm (%)
350	56.3	69.8	66.4
450	63.7	78.5	74.9
600	71.5	87.1	84.2
750	65.8	82.6	80.3

Table 2 shows that nanorod configurations of 80–100 nm have the highest light absorption rates across the entire wavelength range, especially at 600 nm, which is the optimal region for the absorption of medium-energy photons. This structure increases the interaction between photons and the active material, resulting in absorption up to 87.1%, 15% higher than flat structures. This improvement suggests that the vertical orientation of the nanorod expands the optical path of light, increasing the number of photons absorbed before being reflected off the surface.

Surface Morphological Characterization

Table 3. Morphological Parameters of SEM and TEM Analysis Results

Sample	Average Crystallite Size (nm)	Porosity (%)	Surface Roughness (nm)
Flat Structure	45.2	21.5	12.8
Nanorod 80–100 nm	93.7	34.2	28.5
Nanorod >100 nm	112.3	29.7	25.9

Based on morphological analysis, nanorods measuring 80–100 nm have the highest porosity (34.2%) and surface roughness that are ideal for increasing the contact area between the active material and the charge transport layer. Higher porosity values allow for greater light absorption as well as accelerate electron transport. However, an increase in size above 100 nm decreases efficiency as electron transport distances become longer, increasing the risk of charge recombination. This condition strengthens the relationship between microstructures and photovoltaic efficiency.

Electromagnetic Field Distribution Simulation (FDTD)

Table 4. Optical Field Intensity at the Nanorod Focal Point

Configuration	Maximum Field (V/m)	Average Intensity (a.u.)	Dominant Absorption Zone (nm)
Flat Structure	2.1×10^5	0.62	500–600
Nanorod 80–100 nm	3.4×10^5	0.87	550–700
Nanorod >100 nm	3.0×10^5	0.80	550–700

The results of the FDTD simulation show that the 80–100 nm nanorod structure produces the highest optical field intensity, signaling a local increase in photon capture. A more even distribution of the field in the active layer helps to increase the number of electrons that are excited. This is directly correlated with the increase in short-circuit current density (Jsc) measured in experimental tests. In other words, this configuration maximizes the efficiency of photon–electron interactions, thus supporting higher conversion efficiency results.

Statistical Analysis of Efficiency and Morphological Correlation

Table 5. Statistical and Correlation Analysis Results

Parameter	R^2	p-value	Correlation (r)
Nanorod Size vs Efficiency	0.91	<0.01	0.95
Porosity vs Jsc	0.88	<0.05	0.89
Surface Roughness vs Voc	0.79	<0.05	0.84

Statistical analysis showed a strong positive relationship between nanorod size and energy conversion efficiency with a correlation value of $r = 0.95$ and a significance of $p < 0.01$. This suggests that morphological changes, especially in size and porosity, have a direct influence on efficiency improvement. An R^2 value of 0.91 indicates that more than 90% of the efficiency variation can be explained by differences in nanorod structure. Thus, surface morphology is a key factor that determines the performance of TiO_2-based photovoltaic systems.

DISCUSSION

The results of this study show that the increase in energy conversion efficiency in nanostructure-based solar cells is a direct consequence of surface morphological modifications that increase photon–electron interactions. The structure of TiO_2 nanorods measuring 80–100 nm has been shown to have higher light absorption capabilities than flat films, which significantly increases the active surface area for electron transfer. This phenomenon shows that the optimization of nanomaterial geometry not only impacts optical absorption, but also on increased current density (Jsc) and open circuit voltage (Voc). These findings are in line with the view of Chen et al. (2023) who stated that vertically oriented nanostructures are able to amplify the resonance of plasmonic surfaces, thereby improving the efficiency of photon capture in perovskite-based photovoltaic devices.

The main findings of this study confirm that the role of nanorods in strengthening charge transfer pathways is a key factor in improving energy conversion efficiency. The test results showed that the increase in efficiency of up to 23.4% was not only affected by increased absorption, but also by reduced electron–hole recombination due to increased crystallinity of the active layer. This condition reinforces the electron transport theory put forward by Patel et al. (2022), that electron mobility increases significantly when the orientation of the nanostructure is parallel to the conductive substrate. In this context, TiO_2 nanorods serve as transport channels that reduce internal resistance and speed up the charge extraction process, resulting in a more stable increase in total power output.

In addition, the results of finite-difference time-domain (FDTD) simulations show that nanostructures with a diameter of 80–100 nm produce a

more homogeneous distribution of electric fields compared to larger structures. The uniform distribution of the field allows for increased photon absorption effectiveness across the surface of the active layer. These findings are consistent with the report of Wu et al. (2024) which confirms that the regulation of the size and orientation of nanostructures has a direct influence on the local intensity of the optical field as well as the efficiency of the conversion of photon energy into electrons. Thus, the results of the FDTD simulation in this study not only validate the results of the experiment, but also strengthen the understanding of the mechanism of opto-electronic interaction in TiO_2–perovskite-based photovoltaic materials.

Other factors that contribute to determining the optimal performance of nanostructural solar cells are the regularity of the layer morphology and the level of surface roughness. Based on the results of SEM and TEM micrograph analysis, the uniform surface of the nanorod results in better contact between the TiO_2 and perovskite layers, which implies higher electron injection efficiency. This supports the results of the research of Alam et al. (2023), who stated that increased morphological regularity can reduce interface barriers and accelerate charge transfer between layers. Thus, these results show that the nanorod structure not only strengthens the optical effect, but also contributes to the stability and long-term service life of photovoltaic devices.

Theoretically, this research makes an important contribution to the development of nanostructure-based photovoltaic material design concepts. The results of the study expand the classical theory of photon–electron conversion by emphasizing the importance of the role of morphological parameters and surface resonance in optimizing energy absorption. This approach is in line with the opto-electronic model developed by Das & Iqbal (2024), which asserts that precise control of the size and orientation of nanostructures can improve internal quantum efficiency without the need for precious metal-based additives. Thus, this study enriches the literature on nanomaterial engineering strategies for high efficiency and low cost in modern renewable energy systems.

However, this study has some limitations that need to be considered. Particle size variations are still within a small laboratory range, so generalization of results to an industrial scale needs to be studied further. In addition, the use of the FDTD method with certain optical idealization parameters may cause deviations from real conditions. This is similar to the note from Li & Torres (2021) which emphasizes that numerical simulations often do not fully represent optical losses due to interface imperfections. Therefore, further research is recommended to integrate multi-layer experimental approaches and multi-physics numerical models so that the results obtained are more representative of the actual operational conditions of solar cells.

Practically, the results of this study have major implications for the development of efficient and sustainable solar energy technology. The vertically-oriented nanostructure design with controlled size offers great potential for application in the production of low-cost, high-performance solar cells. This strategy enables increased efficiency without reliance on expensive materials, while supporting global clean energy transition targets. In line with the

International Energy Agency (IEA, 2024) report, nanomaterial-based innovations are expected to reduce the cost of solar energy production by up to 30% in the coming decade. Thus, this research not only makes a theoretical contribution to the science of photovoltaic materials, but also provides a strategic direction for the development of renewable energy that is efficient, economical, and environmentally friendly.

CONCLUSION AND RECOMMENDATION

This study shows that the regulation of nanostructures in photovoltaic materials can significantly improve the ability of solar cells to convert light energy into electricity. The 80–100 nm TiO_2 nanorod structure has been shown to improve conversion efficiency by up to 23.4%, higher than conventional flat structures. This increase occurs due to a larger surface area, more optimal light absorption, and reduced electrical charge loss. These results prove that the shape, size, and arrangement of nanoparticles have a significant effect on light capture and electron transfer speed, making it an important basis for the development of TiO_2–perovskite-based photovoltaic technologies in the future.

In practical terms, these findings confirm that nanostructure engineering plays an important role in improving photon–electron interactions and reducing energy loss, thus making a scientific contribution to the development of new generation photovoltaic materials and offering tangible benefits for improving the performance of efficient, low-cost, and environmentally friendly solar cells. In addition, the results of this study provide strategic direction for the development of renewable energy systems that are more sustainable and adaptive to the global need for efficient and environmentally safe energy sources.

FURTHER STUDY

Based on these conclusions, future research should focus on deepening the understanding of how nanostructure configurations influence long-term stability and large-scale applicability of TiO_2–perovskite photovoltaic systems. Further studies are needed to explore alternative nanostructure geometries—such as hierarchical, branched, or multi-layered architectures—to determine their potential for even higher light-harvesting efficiency and faster electron transport. Investigations into the integration of dopants or hybrid nanomaterials could provide insights into enhancing charge mobility and reducing recombination losses under varying environmental conditions. Additionally, future work should examine the durability of these nanostructures under real-world operational stresses, including humidity, temperature fluctuations, and prolonged UV exposure, to ensure reliable performance over time. Expanding this research toward scalable fabrication techniques and cost-efficient production methods will also be essential for enabling commercial adoption. Overall, these further studies will strengthen the scientific foundation for next-generation photovoltaic technologies and support the development of highly efficient, stable, and environmentally sustainable solar energy systems.

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