IOSR Journal of Business and Management (IOSR-JBM)
e-ISSN:2278-487X, p-ISSN: 2319-7668. Volume 27, Issue 11. Ser. 5 (November. 2025), PP 36-46
www.iosrjournals.org

Scientific Advances in Titanium Dioxide (TiO_2)-Based Photovoltaic Cells

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Abstract:
Background: *This article presents a comprehensive review of the use of titanium dioxide (TiO_2) in photovoltaic cells, focusing on its structural, optical, and electronic properties. The study critically examines doping strategies (such as the incorporation of Nb) and morphological modifications, as well as synthesis methods and characterization techniques that influence the performance of TiO_2-based photovoltaic devices, including dye-sensitized solar cells (DSSCs) and perovskite solar cells.*
Materials and Methods: *The review draws on bibliographic prospecting and comparative analysis of recent scientific literature. It discusses various synthesis and characterization techniques—such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV-Vis spectroscopy—used to assess the crystalline structure, optical behavior, and electrical properties of TiO_2.*
Results: *The findings indicate that the field of TiO_2-based photovoltaics is both consolidated and expanding, as evidenced by a growing number of recent publications dedicated to optimizing this semiconductor. Advances in material engineering, synthesis control, and device architecture have contributed to improving the conversion efficiency and stability of solar cells.*
Conclusion: *This study analyzes recent scientific progress in TiO_2-based photovoltaic cells, emphasizing the evolution of materials, manufacturing methods, and energy efficiency improvements. The results highlight the material's potential to support the development of sustainable solar energy conversion technologies. In summary, the research quantifies the impact of different TiO_2 modification approaches on solar cell performance, particularly in enhancing energy conversion efficiency.*

Keywords: *Titanium Dioxide; Photovoltaic Cells; Perovskite; Material Characterization.*

Date of Submission: 12-11-2025 Date of Acceptance: 23-11-2025

I. Introduction

Titanium dioxide (TiO_2) has emerged as one of the most significant semiconductors in the development of photovoltaic technologies within the current context of energy transition. Its low cost, natural abundance, high chemical stability, and favorable electronic properties make it a strategic material for dye-sensitized solar cells (DSSCs) and perovskite solar cells—both considered promising alternatives for the generation of clean and high-efficiency energy.

Despite these intrinsic advantages, TiO_2 exhibits limitations that affect its photovoltaic performance, particularly its wide band gap (approximately 3.2 eV in the anatase phase) and high charge recombination rate. These factors restrict its light absorption in the visible region of the solar spectrum and limit the energy conversion efficiency of devices. Such challenges have driven the search for advanced materials engineering solutions, emphasizing doping strategies and nanostructuring approaches to improve light absorption, charge separation, and carrier transport.

This research was developed through bibliographic prospecting and comparative analysis, revealing a consolidated and expanding scientific field, with a substantial number of recent publications focused on optimizing this semiconductor. The main objective of this study is to analyze recent scientific advances in TiO_2-based photovoltaic cells, focusing on material evolution, fabrication methods, and improvements in energy efficiency, aiming to understand their potential contribution to the development of sustainable solar energy conversion technologies.

The specific objectives are as follows: To analyze the different crystalline phases of titanium dioxide (anatase, rutile, and brookite) and their influence on structural properties and photovoltaic performance; To investigate the effects of metallic and non-metallic dopants on the electronic properties of TiO_2 and evaluate how such modifications contribute to enhancing solar energy conversion efficiency; To examine major morphological modification and nanoengineering approaches applied to TiO_2 to improve active surface area, charge mobility, and electronic transport in photovoltaic devices; To describe and compare the most common synthesis methods for TiO_2 nanomaterials—such as sol-gel, hydrothermal, and sputtering—emphasizing their implications for structure and material properties; To evaluate the main structural and morphological characterization techniques applied to TiO_2, including X-ray diffraction (XRD) and scanning electron microscopy (SEM), highlighting their importance for understanding the material's physicochemical behavior; To investigate the optical behavior of TiO_2 through UV-Vis spectroscopy, analyzing the influence of structural and electronic modifications on light absorption and photovoltaic conversion efficiency.

The article is organized into five sections. The first section introduces the study and outlines its objectives. The second, *Materials and Methods*, explains the methodological procedures adopted for the research. The third, *Theoretical Framework*, discusses the main studies addressing similar topics. The fourth section presents and discusses the results, synthesizing and comparing key findings from recent literature to identify trends, gaps, and prospects for developing more efficient and sustainable photovoltaic technologies. Finally, the fifth section contains the *Concluding Remarks*.

II. Material And Methods

The scientific prospecting was carried out using the databases Google Scholar, CAPES Journal Portal, EBSCOhost, SciELO Brazil, and the UNIFOR integrated journal search platform, employing the keywords *"photovoltaic solar cells"* and *"titanium dioxide."* The research followed the methodological principles described by Barros and Porto Junior (2021), considering technological prospecting as a tool for the analysis and systematization of scientific knowledge.

The search encompassed publications in different languages, with filters covering the period from 1984 to 2025, and included only peer-reviewed articles. Duplicate and redundant studies were excluded, resulting in a consistent corpus for analysis. The collected data were organized into charts and tables to provide a clear visualization of the identified trends and correlations. Subsequently, the information was scientifically analyzed and discussed, aiming to relate the observed advances to the technological development of TiO_2-based photovoltaic cells.

III. Literature Review

Titanium dioxide (TiO_2) exhibits three primary crystalline phases: anatase, rutile, and brookite. Among these, the anatase phase is the most commonly employed in photovoltaic devices due to its favorable band gap, high photoelectrochemical activity, and efficient charge separation. The optimization of its electrical, optical, and structural properties has been extensively explored through doping and nanoengineering strategies.

3.1 Structure and Crystalline Phases

The polymorphism of TiO_2 has a direct influence on its photovoltaic performance. The anatase phase presents a band gap of approximately 3.2 eV, higher than that of rutile (3.0 eV), but offers superior charge separation efficiency and better photoelectrochemical performance. Structural characterization is essential to understanding these properties, and Rietveld refinement is recognized as a highly rigorous technique for determining phase proportions, crystallite size, and microstrains—factors that directly affect the efficiency of photovoltaic devices.

3.2 TiO_2 Doping Strategies

Doping represents a widely investigated approach to enhance the optical absorption, charge mobility, and photovoltaic performance of TiO_2. The introduction of metallic cations such as Nb, Sn, Zr, and Ta increases conductivity and facilitates electron transport, leading to improved conversion efficiency. Rare-earth ions (Eu^{3+}, Tb^{3+}, Yb^{3+}) have been explored for their ability to enhance luminescence and energy conversion. Nonmetallic doping, such as with nitrogen, shifts light absorption toward the visible region, improving solar spectrum utilization.

3.3 Morphological Modifications and Nanoengineering

Morphological engineering techniques contribute to increasing the surface area, improving electronic mobility, and optimizing active interfaces. Electrochemical anodization enables the formation of vertically aligned TiO_2 nanotubes that promote efficient electron transport. Other morphologies, such as nanorods, nanowires, and oriented thin films, have demonstrated significant performance gains. The construction of heterostructures with semiconductor oxides such as ZnO, CuO, or NiO allows for the exploration of functional synergies that enhance charge separation and transport.

3.4 Synthesis Techniques for TiO_2-Based Materials

Several synthesis routes have been developed to obtain TiO_2 nanostructures and thin films for photovoltaic applications. The main techniques include:

- **Sol-Gel Method:** Enables precise control of composition and morphology, widely used for producing TiO_2 doped with metallic and rare-earth ions.
- **Electrodeposition:** Applied to the formation of nanostructured films, often adapted to oxides such as ZnO and TiO_2.
- **Magnetron Sputtering:** Allows controlled deposition of TiO_2 films with adjustable density and refractive index depending on the incidence angle.
- **Spray Pyrolysis:** A cost-effective, scalable technique commonly used for depositing compact TiO_2 layers on transparent conductive substrates.
- **Atomic Layer Deposition (ALD) and Chemical Vapor Deposition (CVD):** High-precision methods for obtaining ultrathin, uniform layers essential to perovskite devices.

3.5 Material Characterization Techniques

The structural, optical, and photoelectrochemical evaluation of TiO_2 and related devices involves a range of characterization techniques, as summarized in **Table 1**.

Table 1 - *Main characterization techniques applied to TiO_2-based materials*

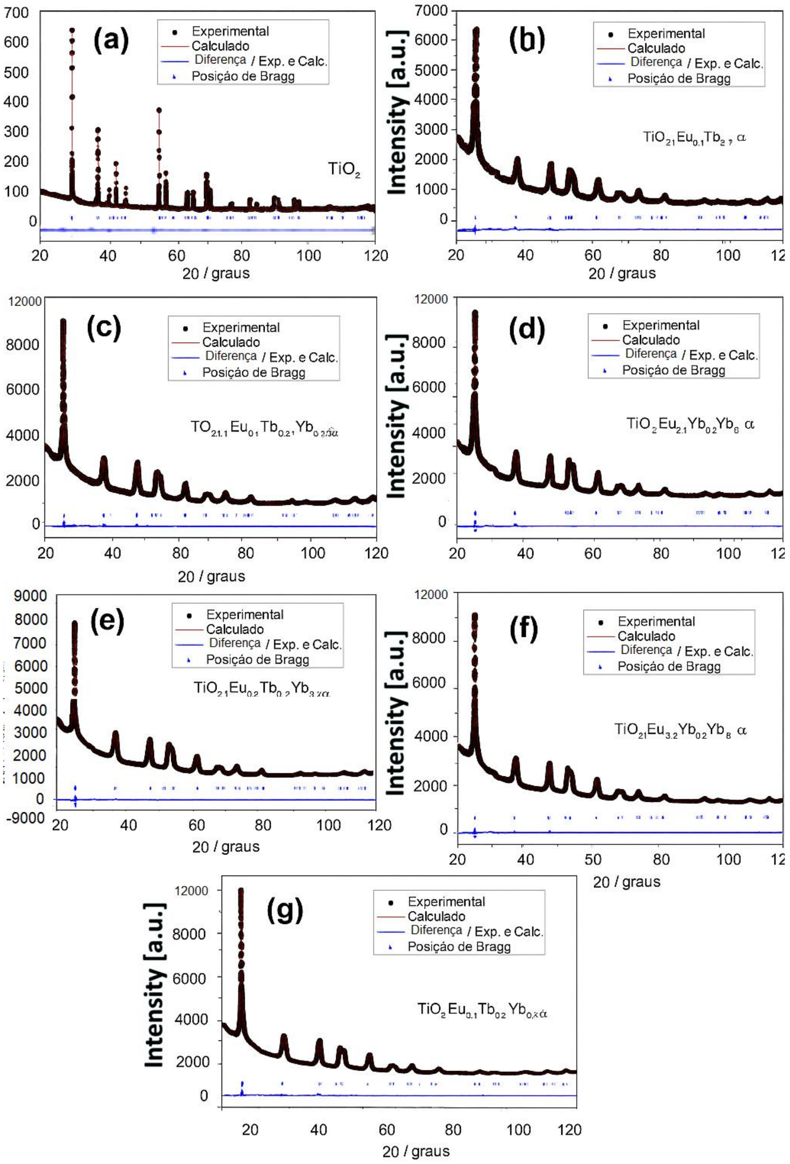
Category	Techniques	Objective
Structural	XRD, SEM, TEM, Raman	Identification of phases, morphology, and crystallinity
Optical	UV-Vis, Photoluminescence	Band gap, absorption, and electronic transitions
Electrical and Photoelectrochemical	I–V, EIS, Cyclic Voltammetry	Evaluation of efficiency, recombination, and charge transport

Source: Researchers' Data

The diffractogram in **Figure 1** shows the induction of crystallization from the amorphous TiO_2 structure, demonstrating how crystallite size and microstructural charge transfer modulations are essential for quantifying structural parameters through Rietveld refinement. The results also indicate that the detection of peaks at specific angles, similar to those reported by Oliveira et al. (2024), such as the (101) peak for anatase in Nb-doped TiO_2: Nb films, can validate the formation of a structure favorable for photocatalytic and photovoltaic applications, ensuring stability in the anatase phase.

As observed in films doped with TR^{3+} ions, a decrease in the (101) peak intensity may indicate difficulty in incorporating the ions into the host matrix or changes in crystallinity (Wang et al., 2015, p. 154). Therefore, Rietveld refinement provides critical parameters for optimizing charge transfer and device efficiency, using crystallite size and microstrain as quantification metrics.

Figure 1 – X-ray diffraction patterns of pure and rare-earth-doped TiO_2 films.

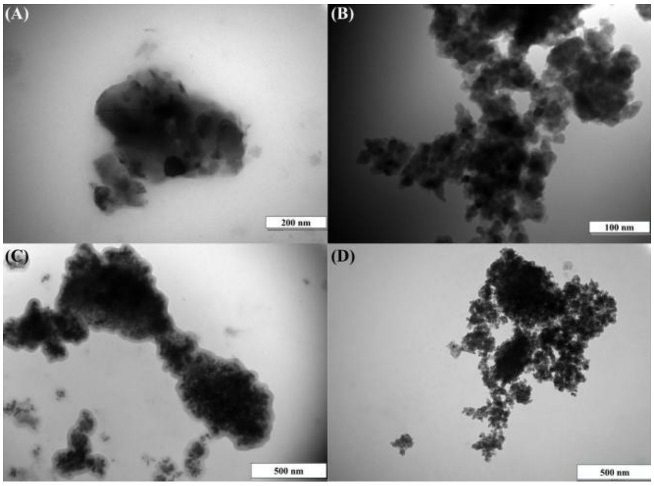


Source: Carneiro (2024, p. 30)

In **Figure 2**, by analogy, scanning electron microscopy (SEM) images (Carneiro, 2024) are presented, which are essential for visualizing the surface morphologies of TiO_2 films, as they reveal rare-earth-doped TiO_2 nanostructures. The images include micrographs obtained by SEM and transmission electron microscopy (TEM) for analyzing particle size distribution, morphology, and the estimation of average crystallite size in TiO_2 samples doped with TR^{3+} ions. These samples were produced via the sol-gel method and thermally treated at 700 °C for eight hours: (A) TiO_2, (B) TiO_2: Eu 3%, Tb 0.04%, (C) TiO_2: Eu 3%, Tb 0.04%, Yb 0.5%, and (D) TiO_2: Eu 3%, Tb 0.04%, Yb 1.5%. This process allows for a direct correlation between synthesis conditions and the resulting nanostructure.

The oblique angle deposition (OAD) technique can reveal that films with lower density and refractive index tend to decrease as the deposition angle increases (Alba-Cabañas, 2025, p. 41). In **Figure 2**, the homogeneous formation of TiO_2 nanotubes can be observed, showing well-distributed particles following the anodization process. Moreover, SEM images enable the examination of compact layers, allowing the identification of uniformity, defects, or agglomerates that may compromise or potentially affect the performance of the device.

Figure 2 – Scanning Electron Microscopy (SEM) images of TiO_2 nanostructures.



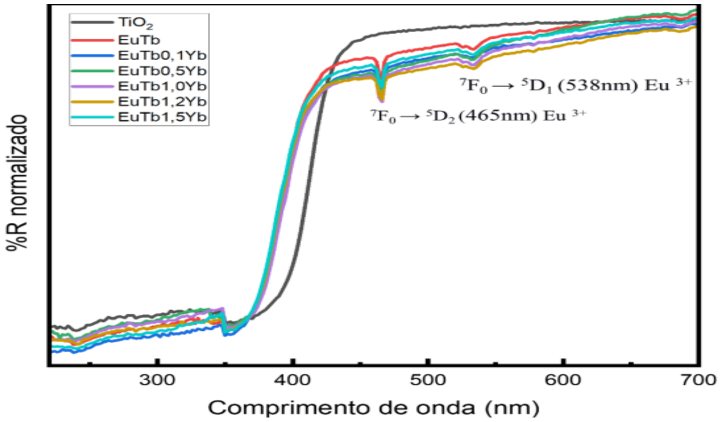
Source: Carneiro (2024, p. 39)

3.6 Optical Characterization (UV-Vis)

In **Figure 3**, diffuse reflectance spectra are shown, corresponding to **Figure 4.10** in Carneiro (2024, p. 46). The UV-Vis spectroscopy results allow for the determination of the optical band gaps of each material, as illustrated in the same study (Carneiro, 2024, p. 47). It can be observed that doping with niobium or rare-earth ions affects the modulation of the TiO_2 band gap, resulting in more efficient light absorption in the visible region.

In the ZnO:N films, the band gap values between 3.34 and 3.17 eV depend on the calcination conditions (Silva, M. K., 2023, p. 54). Therefore, the crystalline phase transition from rutile to anatase, as indicated by Carneiro (2024, p. 48), suggests that doping may account for the increase in band gap energy. In other words, in compact TiO_2 layers, the transmittance spectrum shows a decrease in transmittance percentage as the number of layers increases, which consequently alters the film thickness.

Figure 3 – UV-Vis Transmittance Spectra of pure and TR^{3+}-doped TiO_2 films.



Source: Carneiro (2024, p. 46)

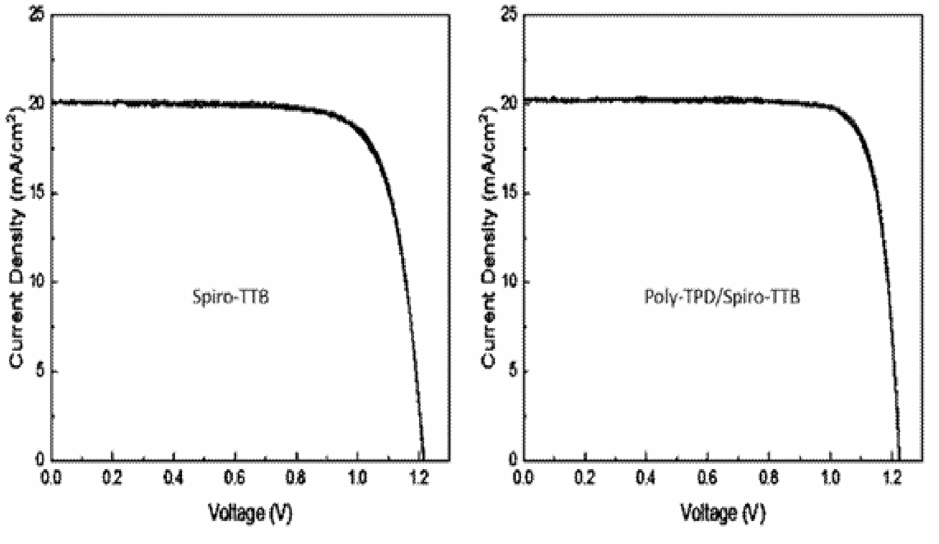
3.7 J–V Curves and Photocurrent Analysis

The J–V curves (photocurrent density versus voltage) are essential for evaluating the performance of solar cells. **Figure 4** presents the photochronoamperometric curves for TiO_2 and TiO_2:Nb systems (AU 2023250513 A1, 2023; Oliveira et al., 2024). Niobium (Nb) doping leads to a significant increase in short-circuit current density (Jsc) and conversion efficiency (η), as reported by Oliveira et al. (2024).

This improvement, which raised efficiency from 32.11% to 66.84%, is intrinsically related to the modulation of TiO_2's electronic properties, optimizing charge collection. The obtained values show an increase in Jsc from 0.1404 $mA\cdot cm^{-2}$ to 0.2036 $mA\cdot cm^{-2}$. To minimize electron back transfer and further enhance Jsc and the fill factor (FF) in DSSCs, it is necessary to optimize the interface using Electrochemical Impedance Spectroscopy (EIS) analysis (Oliveira et al., 2024).

Optimizing transport layers and potential barriers requires reducing carrier recombination by achieving higher Jsc and Voc values. This outcome supports the potential of doping to enhance charge collection and overall device efficiency, as demonstrated in perovskite cells from patent AU 2023250513 A1 (2023). Furthermore, "using an additional compact TiO_2 layer in DSSCs can increase Voc and the fill factor (FF), thereby mitigating electron back transfer" (Alba-Cabañas, 2025, p. 27).

Figure 4 – J–V Curves of TiO_2: Nb-sensitized solar cells, Figures 4(a) and 4(b).



Source: WO 2023/193065 – PCTAU2023/050286 – 16/72 (2023, p. 210)

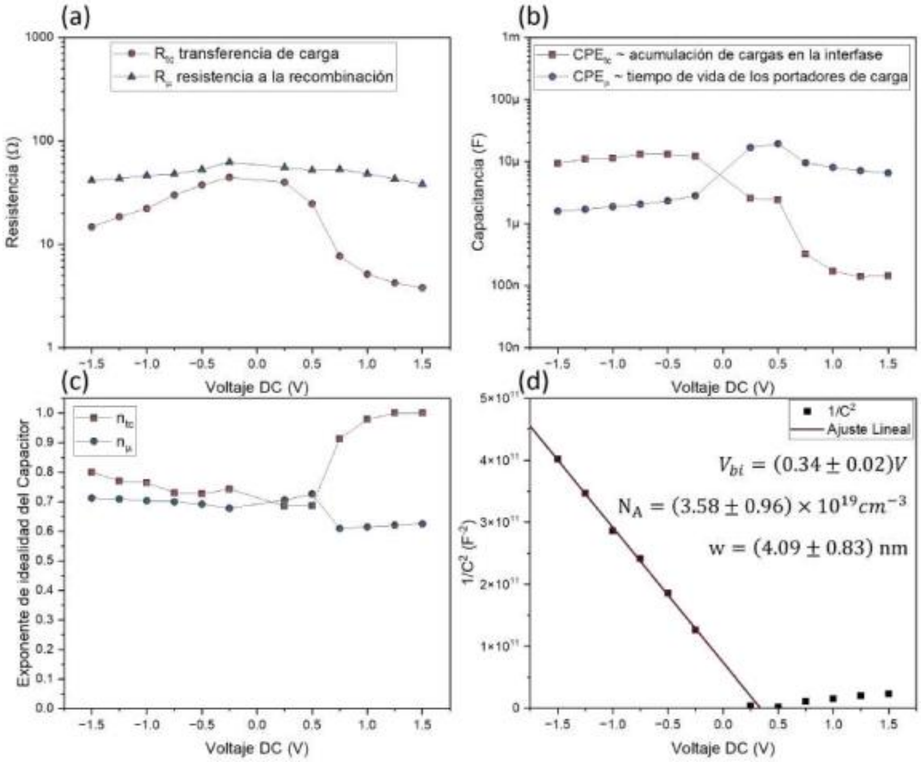
To ensure that the results presented here are interpreted accurately, it is important to clarify that the photovoltaic efficiency values reported in this section refer exclusively to the efficiency measured under the specific controlled conditions established in the study, rather than to internal metrics such as external quantum efficiency or normalized photocurrent (Green et al., 2023).

3.8 Mott–Schottky Analysis and Charge Transport Mechanisms

As illustrated in **Figure 5**, the Mott–Schottky analysis, derived from Electrochemical Impedance Spectroscopy (EIS) and applied to the ZnO, CuO, and NiO heterostructure, is essential for elucidating the transport and recombination mechanisms at the interface. The EIS results confirmed that carrier recombination is the main efficiency-limiting factor and that charge transport in nanostructured devices is predominantly governed by diffusion processes. This indicates that charge transport mechanisms are dominated by diffusion in nanostructured dimensions (Alba-Cabañas, 2025), characterizing an electrochemical (impedance spectroscopic) connection.

To reinforce interface optimization, as proposed in patent **WO 2024118031 A2 (2023)**, it is necessary to minimize charge losses through linear adjustment of the negative slope of the graph, which yielded an intercept of **(0.34 ± 0.02) V**, indicating that carrier injection increases from this value onward. The slope of the line allows the calculation of carrier density, resulting in **$(3.6 \pm 1.0) \times 10^{19}$ cm^{-3}**, a value consistent with those reported in the literature for nanostructured layers (Alba-Cabañas, 2025).

Figure 5 – Mott–Schottky plot for a ZnO/CuO/NiO heterostructure.



Source**:** Alba-Cabañas (2025, p. 85)

Caption**:** (a) *Resistances as a function of voltage:* the resistance associated with contacts and the resistance related to recombination remain constant, while the charge-transfer resistance varies with the voltage direction, showing an abrupt decrease in the positive direction; (b) *Capacitances related to charge transfer and recombination:* the transfer capacitance decreases in the positive direction, while the recombination capacitance varies less markedly; (c) *Capacitor ideality exponent:* the exponent for recombination remains constant, while the charge-transfer exponent increases at voltages above 0.5 V, suggesting improved current distribution; (d) *Determination of internal potential and carrier density* of the system based on the Mott–Schottky model.

The discussion of EIS and the Mott–Schottky plot should extend beyond acknowledging recombination as a critical factor. It is necessary to examine how the obtained carrier density values — **$(3.6 \pm 1.0) \times 10^{19}$ cm^{-3}** — compare with ideal limits, and how diffusion within nanostructures constitutes the dominant pathway for charge transport. Furthermore, the explicit relevance of ZnO, CuO, and NiO heterostructures to the performance of multilayer devices must be addressed.

IV. RESULTS AND DISCUSSION

Initially, it is necessary to compare the properties (band gap, photoelectrochemical activity, stability) of the crystalline phases and the main dopants explored, relating them directly to their role in optimizing light absorption or charge transport, as shown in **Table 2**. Doping with rare earth elements (RE^{3+}) highlights that the optimization of luminescence (energy conversion) results from photon up-conversion or down-conversion phenomena, which modulate light absorption in the visible and infrared regions.

In the structural characterization, Rietveld refinement enables not only the quantification of crystallite size but also the percentage of crystalline phases (rutile), which is directly correlated with charge separation efficiency. In the J–V curves, Nb doping increased efficiency from **32.11% to 66.84%**, indicating that this performance enhancement is associated with the creation of oxygen vacancies or an increase in the concentration of free charge carriers (Nb^{5+} substituting Ti^{4+}), which represents the electronic mechanism that **optimizes charge collection**.

Table 2 – Comparative Properties: Crystalline Phases and Dopants of TiO_2 in Photovoltaic Applications

Material / Morphology	Crystalline Phase	Band Gap (Eg) / Measurement in eV	Optical / Structural Characterization	Photoelectrochemical and Charge Transport Properties
Pure TiO_2 (TiO_2)	Anatase	3.2 eV	Stable anatase phase	Semiconductor with high photocatalytic activity; suitable for photovoltaic devices.
Pure TiO_2 (TiO_2)	Rutile	3.0 eV	More stable at high temperatures	Lower charge separation efficiency; recombination occurs more easily.
Doped TiO_2 (TiO_2:Nb)	Niobium (Nb)	Modified band gap (≈ 3.05 eV)	Increased crystallinity; anatase phase maintained	Increased short-circuit current density (Jsc) and efficiency (η); oxygen vacancies improve charge mobility.
Doped TiO_2 (TiO_2:RE^{3+})	Rare Earth Ions (Eu^{3+}, Tb^{3+}, Yb^{3+})	Modified band gap depending on dopant	Photoluminescence up-conversion or down-conversion phenomena	Enhanced light absorption in visible and IR regions; improved electron-hole separation.
Doped TiO_2 (TiO_2:TR^{3+} + Nb)	Mixed dopants (RE^{3+} + Nb^{5+})	Band gap adjusted by co-doping	Improved structural order; reduced recombination	Synergistic effect between optical conversion and charge collection; higher efficiency.
ZnO-based Heterostructures (ZnO/CuO/NiO)	Multilayer Oxides	3.3 – 3.17 eV (depending on calcination)	Mott-Schottky and EIS characterization	Dominant charge transport by diffusion; recombination identified as limiting factor; increased internal potential and carrier density.

Source: Researchers' Data

Regarding EIS and Mott–Schottky analysis, the carrier density of $(3.6 \pm 1.0) \times 10^{19}$ cm^{-3} can be compared with typical values reported for pure TiO_2 in the literature, allowing for an assessment of whether the ZnO, CuO, and NiO heterostructure achieved the expected level of interface engineering for multilayer devices. The fact that the carrier density is consistent with the literature values for nanostructured layers, combined with the observed reduction in interfacial charge losses (the main goal of the heterostructure), suggests that the interface engineering reached a satisfactory level of optimization in the context of multilayer devices. If TiO_2 were employed as a single layer, this value would be compared to the ideal standard. However, since it is part of a heterostructure, the measured value reflects the combined efficiency of the layers in carrier injection and transport, which represents a positive outcome.

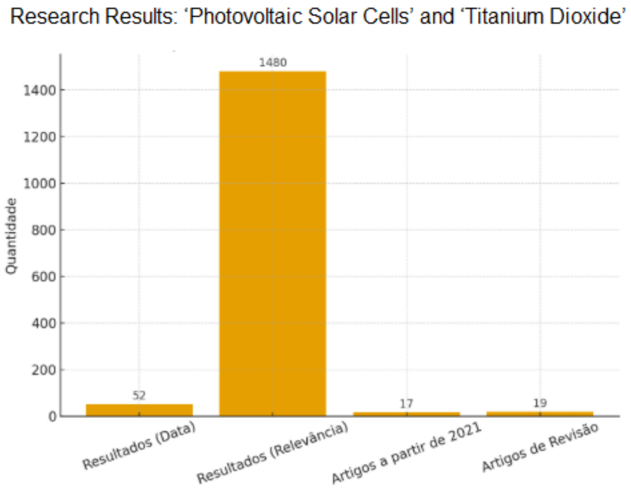
In the Mott–Schottky plot for a ZnO/CuO/NiO heterostructure (**Figure 5**), the analysis demonstrates the ability to distinguish between resistances and capacitances, separating the resistance associated with recombination (which remains constant with respect to voltage) from the charge transfer resistance (which varies). This distinction allows for a detailed evaluation of how charge transfer capacitance decreases in the positive bias direction compared to recombination capacitance, which changes less significantly. Therefore, EIS not only confirms the presence of recombination but also provides quantitative parameters—resistance, capacitance, and carrier density—that enable researchers to design optimized interfaces for improved device efficiency.

These findings are supported by scientific studies that identified similar patterns in the current technological literature and databases on this topic.

4.1 Google Scholar

Using the keywords *"photovoltaic solar cells"* and *"titanium dioxide"*, 52 results were found when sorted by date and 1,480 by relevance. Among these, 17 articles were published after 2021, including 19 review papers, as shown in **Figure 6**.

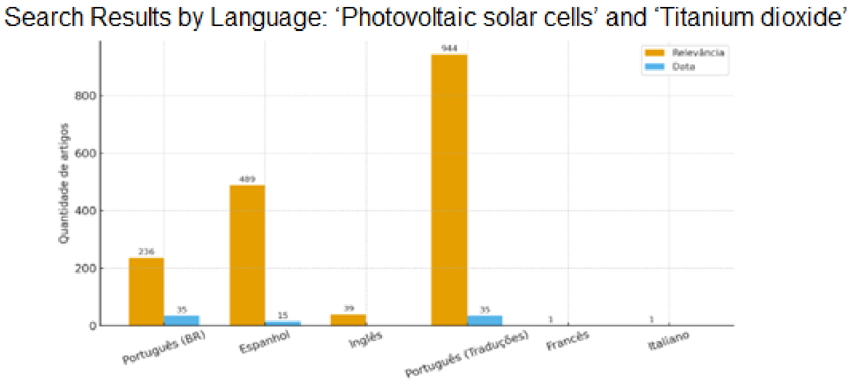
Figure 6 – Prior Art Search Chart for Scientific Articles



Source: Researchers' Data

When restricting the search to Brazilian Portuguese, 236 results were obtained by relevance and 35 by date. In Spanish, 489 articles were identified by relevance and 15 by date. In English, 39 articles were found by relevance and none by date. For translations into Portuguese, 944 were retrieved by relevance and 35 by date. In French and Italian, one result was found by relevance and none by date, as shown in **Figure 7**. No publications were identified in Turkish, German, Dutch, Japanese, Polish, Chinese, or Korean.

Figure 7 – Search Results for Scientific Articles by Language

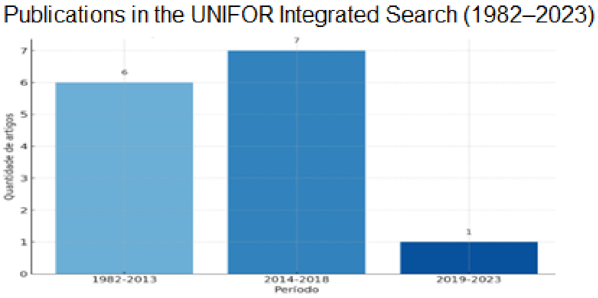


Source: Researchers' Data

4.2 CAPES Journal Portal and UNIFOR Integrated Search Database

In this database, only one article was found: FONSECA, F. J.; ANDRADE, A. M.; FLACKER, A. (1985). *Titanium dioxide films for use in photovoltaic conversion deposited by reactive bombardment. Revista Brasileira de Aplicações de Vácuo.* The Integrated Journal Search of the UNIFOR Central Library identified 14 articles published between 1982 and 2023, with a higher concentration between 2014 and 2018 (seven publications). All of them are indexed and linked to Google Scholar and Scopus, as shown in **Figure 8.**

Figure 8 – Results of the scientific article search

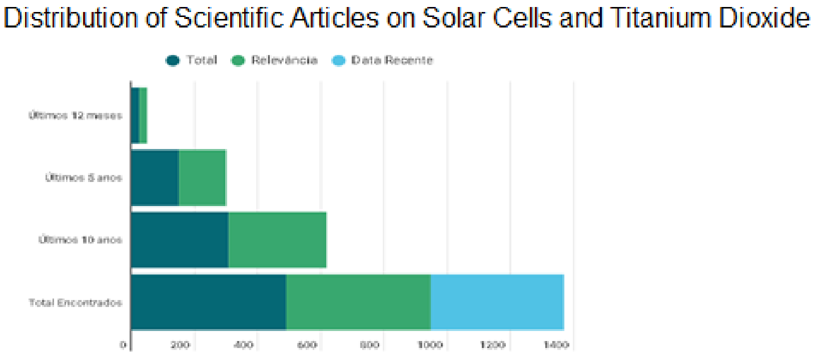


Source: Researchers' Data

4.3 EBSCOhost

With access to 27 databases, 489 scientific articles were identified, 458 ranked by relevance and 420 by most recent date. Among these, 24 publications were released within the past 12 months, 149 in the last 5 years, and 308 in the last 10 years, indicating a consolidated and active research field, as shown in **Figure 9**.

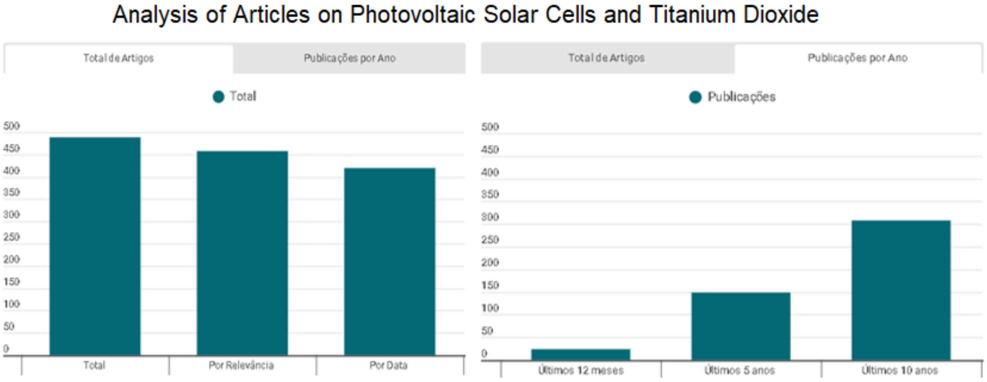
Figure 9 – Search results for scientific articles on EBSCOhost



Source: Researchers' Data

Another option for Figures 10A and 10B – by relevance and by year.

Figure 10 – Results of the scientific article search – by relevance and by year.



Source: Researchers' Data

Searches for scientific articles revealed a significant number of publications, particularly in Portuguese and Spanish, with a peak between 2014 and 2018. There is a substantial body of easily accessible scientific production in databases across other languages. Advances in the use of TiO_2 are not limited to photovoltaic panels and cells; a wide range of scientific studies highlight its applications, possibilities, benefits, and limitations in several other fields beyond the photovoltaic domain.

IV. Conclusion

This prospective research reflects the critical synthesis of results in proposing future pathways and the vast potential of titanium dioxide (TiO_2) as a fundamental material for the next generation of photovoltaic technologies. The integration of doping strategies (with niobium, rare earth elements, or other metal cations) and the optimization of nanostructured morphologies (nanotubes, compact layers) can drive significant advances in the efficiency and stability of solar cells.

Scientific evidence demonstrates the high scientific value of the synergistic integration of specific Nb dopants and TiO_2 with high surface area nanostructures (nanotubes), with the validation of efficiency gains performed by in operando characterization (EIS) to consolidate TiO_2 as an essential material. Similarly, doping strategies, morphological control, and advanced deposition techniques are crucial in overcoming limitations related to stability and efficiency.

Continuous progress in this field requires the mechanistic validation of efficiency gains through in operando characterization techniques, such as EIS, to quantify and mitigate recombination losses at nanostructured interfaces, thereby consolidating titanium dioxide (TiO_2) as a key material for emerging next-generation solar cells. The ongoing scientific advancement in this area is vital for establishing sustainable solar technologies.

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