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Synthesis and Characterization of Titanium Dioxide-Based Nanocomposites for Visible-Light-Driven Degradation of Emerging Organic Contaminants

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Abstract--- Emergence of various organic compounds as emerging contaminants in water bodies has increased the demand for wastewater treatment techniques. Existing wastewater treatment methods might not remove pharmaceuticals, pesticides, dyes, and other persistent organic compounds. Titanium dioxide (TiO_2) has been widely researched in terms of its photocatalytic properties. However, the wide band gap of TiO_2 and the fast recombination of electrons and holes reduce the efficiency of TiO_2 under visible light irradiation. This work offers to synthesize and characterize TiO_2-based nanocomposites for efficient visible light-mediated degradation of organic contaminants. Novelty of the suggested research includes preparation of the modified TiO_2 nanocomposites with enhanced properties related to visible light absorption, separation of charges, and photocatalytic activity. Proposed methodology includes synthesis and characterization of nanocomposites with the help of XRD, SEM, TEM, FTIR, UV–Vis DRS, PL, and BET methods. Photocatalytic studies will include the study of contaminant degradation through the use of visible light radiation by analyzing the factors like catalyst concentration, pollutant concentration, exposure period, and solution pH. The efficiency of degradation, reaction kinetics, and mineralization will be analyzed using suitable analysis procedures. From the anticipated results, it can be seen that the modified TiO_2 nanocomposites will exhibit better visible light utilization ability, lower charge recombination rates, and greater contaminant removal ability compared to unmodified TiO_2.

Keywords--- Titanium Dioxide, Nanocomposites, Photocatalysis, Visible Light, Emerging Contaminants, Wastewater Treatment, Nanomaterials, Degradation Kinetics.

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I. Introduction

Organic contaminations of water bodies with persistent organic pollutants are an environmental issue since such pollutants have a prolonged time of existence in aquatic environments, are continually discharged into the water bodies, and can affect ecological systems. Emerging organic compounds from pharmaceuticals, cosmetics, pesticides, and industrial compounds are often found in wastewaters and water bodies. Classical treatment methods like biological treatment, filtration, and chemical oxidation cannot fully remove these pollutants from the wastewater or even accumulate the pollutants in the recipient environment. Hence, modern techniques able to degrade persistent organic compounds are urgently required.

Photocatalysis is an approach that can be applied in water treatment since it uses the energy of light to provide oxidation and reduction of pollutants on the surface of semiconductor compounds (Inamdar et al., 2024; Rex M & Mukherjee, 2022). Titanium dioxide (TiO_2) is studied extensively due to its chemical inertness, low cost, photocatalytic properties, and environmentally friendly nature (Anirudhan et al., 2020; Morante et al., 2025; Liao et al., 2020). Nevertheless, classical TiO_2 is limited due to UV-dependent activation, narrow range of visible light usage, and high recombination rate of photogenerated charge carriers (Wei et al., 2023).

The synthesis of nanocomposites based on TiO2 provides an avenue to address these issues using material modification, heterojunction, and enhanced interface charge transport. The use of suitable semiconductors, carbonaceous materials, and selective metals may be employed in modifying optical and separation of charges. What makes this study novel is the synthesis and characterization of TiO2 nanocomposites and their application

in visible light-driven degradation of emerging organic contaminants (Mao et al., 2024; Tiwari et al., 2024; Tong et al., 2020).

Problem Formulation

The emergence of new organic pollutants in the wastewater stream constitutes a great concern since many of these substances are resistant to traditional treatment techniques and may continue to be present in water bodies. Even though titanium dioxide has been identified as a great photocatalytic semiconductor, the limited absorption of visible light and electron-hole pair recombination have limited its use in normal lighting conditions. In addition, the variability in properties of the pollutants, catalyst composition, chemical properties of the solution, and conditions of operation affect the effectiveness of the degradation process. It is important, therefore, to develop efficient TiO_2 nanocomposites that have enhanced photo properties and stability after multiple treatment cycles.

Study Overview

The rest of the paper is divided into separate sections. In the literature review section, the current trends in TiO_2 photocatalysis and nanocomposites modification will be described, as well as the identification of research gaps. Methodology outlines the method of preparation, characterization, and evaluation of the material for its photocatalytic performance. There are two separate technical sections about material modification techniques and contaminants degradation processes. Results and discussion analyze the expected connection between the material properties and its performance.

II. Review of Relevant Literature

The extensive study of titanium dioxide as a semiconductor photocatalyst for environment remediation is due to its chemical stability, appropriate band structure, lower cost of fabrication, and capacity to form reactive oxygen species upon illumination (Ismael et al., 2020; Nelson et al., 2025). The photocatalysis process of titanium dioxide takes place by the formation of electron-hole pairs as a result of the absorption of photons and the transfer of electrons from the valence band to the conduction band (Krakowiak et al., 2021; Sacco et al., 2021). These charge carriers take part in redox reactions at the surface leading to the formation of reactive species for the decomposition of organic pollutants. However, traditional TiO_2 suffers from limited photocatalytic activity under visible light irradiation due to its wide bandgap and fast recombination of electron-hole pairs. There have been different approaches to modify TiO_2 in order to resolve the above-mentioned issues. Such methods may enhance light harvesting, modify electronic configuration and promote charge transfer at the interface. The formation of heterojunctions based on TiO2 has gained increasing interest since by mixing two appropriate semiconductors, the formation of favorable charge transfer paths can be achieved. Carbonaceous materials like graphene-based materials and carbon nanotubes can help to enhance charge transfer efficiency and also serve as extra adsorption sites. Metals incorporated into nanocomposites can affect optical absorption and charge carrier dynamics. Excessive metal content may lead to the formation of new recombination centers or cover active sites. Contemporary photocatalysis studies tend to give preference to the removal of pharmaceutical waste products, pesticides, dyes, and other emerging contaminants. Typically, experimental assessment includes testing of catalyst efficiency for removing contaminant under controlled irradiation, kinetic analysis and reusability of the catalyst. Characterization tools such as XRD, electron microscopy, FTIR, UV–Vis spectroscopy, and photoluminescence give insights into crystalline structure, morphology, functional groups, optical absorption and charge recombination. However, the differences in experimental conditions and type of pollutants make any comparative analysis hard to conduct. Therefore, comprehensive research is required.

Unaddressed Research Issues

Despite a lot of advancements in TiO_2 photocatalysis, there are some gaps in current researches. Most studies have concentrated on the improvement of absorption of visible light only, whereas charge carriers dynamics, efficiency of mineralization, and stability of the catalyst should be considered together. Moreover, the impact of the composition of the nanocomposites, their interphase interactions, and conditions of synthesis should be investigated in detail. Variations in the experimental lighting, pollution concentration, and chemical solution composition hinder the comparability between the results obtained from different studies. This research will fill this gap through comprehensive structural, morphological, optical, and photocatalytic analysis of samples under experimental conditions.

III. Experimental Procedure

System Architecture

The suggested methodological approach encompasses the integrated experimental procedure which covers nanocomposite synthesis, characterization, and photocatalytic activity assessment. Nanostructured composites based on TiO_2 will be synthesized in accordance with the specific process, where chosen semiconductor or carbon-containing additives will be used to enhance the material's photoactivity in visible range of light. Structural, morphological, chemical, optical, and surface characterization of synthesized materials will be performed. Then photocatalytic experiments will be carried out using chosen organic contaminants in visible light irradiation conditions. Parameters such as catalyst dose, concentration of pollutant, pH of the solution, and duration of irradiation will be varied.

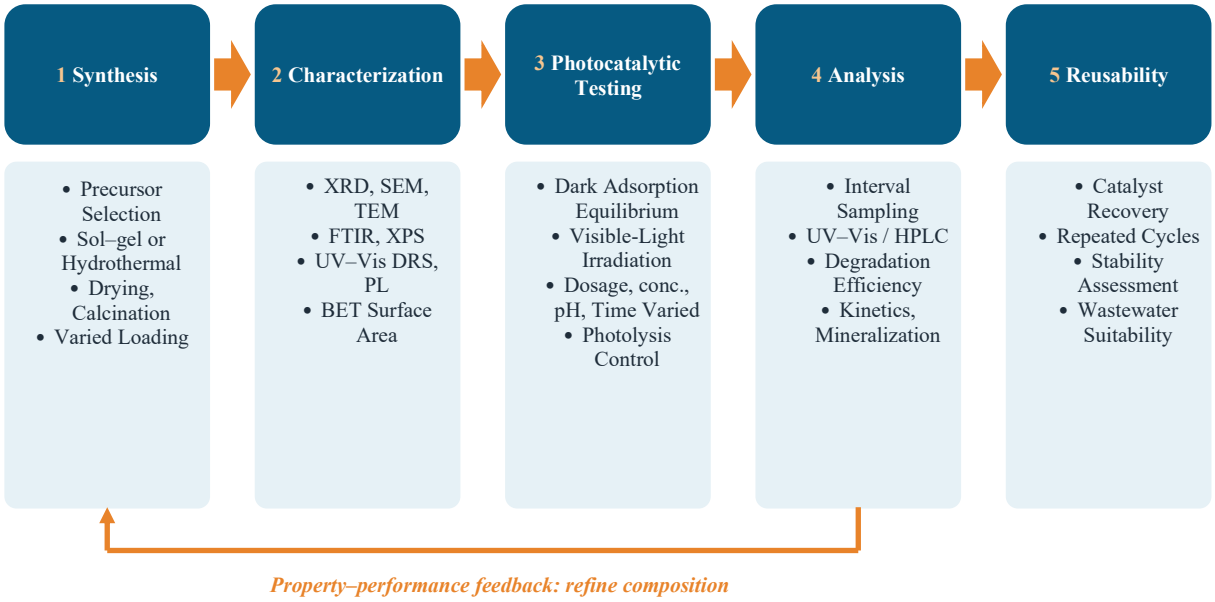


Figure 1: Proposed Methodology Architecture for TiO_2-based Nanocomposite Synthesis and Photocatalytic Degradation

Figure 1 depicts the experimental process that is designed to obtain the visible light active TiO2 nanocomposites. Firstly, the choice of the precursor materials and the synthesis of the materials take place. Afterwards, characterization of the prepared nanocomposites is done in order to understand the structural, morphological, chemical and optical properties of the nanocomposites. The photocatalytic activity tests are done by choosing some organic pollutants under the visible light illumination. Finally, the stability and recyclability of the catalysts are analyzed.

Nanocomposite Synthesis and Preparation

The preparation of the proposed TiO_2-based nanocomposites will utilize a proper sol-gel, hydrothermal, or controlled precipitation method. Precursor of titanium along with the chosen modifying materials will be combined in a suitable temperature, pH, and agitation level. The aged, washed, dried, and calcined product will then be subjected to characterization studies. The modifying material might be either light-responsive semiconductor or carbon. Different amounts of materials will be synthesized in order to study the effect of the load of the material on photocatalytic performance.

Characterization Techniques

The characterization methods for TiO_2-based nanocomposites are summarized in table 1 below. The mentioned methods assess crystalline structure, morphology, particle size, functional groups, optical behavior, charge recombination, surface area, and chemical composition.

Table 1: Characterization Techniques and Their Purposes for TiO_2-Based Nanocomposites

Technique	Purpose
XRD	Crystal Structure and Phase Identification
SEM	Surface Morphology
TEM	Particle Size and Internal Structure
FTIR	Functional Groups and Chemical Bonding
UV–Vis DRS	Optical Absorption and Estimated Band Gap
Photoluminescence	Electron–Hole Recombination Behavior
BET	Specific Surface Area and Pore Characteristics
XPS	Surface Chemical Composition and Oxidation States

Photocatalytic Experimental Procedure

Selected examples of emergent organic pollutants, for instance pharmaceuticals or artificial dyes, will be selected as model pollutants. A certain amount of the photocatalyst will be dispersed into the solution containing the pollutant. Prior to illumination, the mixture will be kept in darkness in order to reach equilibrium of adsorption-desorption process. Afterwards, visible light will be applied. Samples will be collected at certain time points, separated from catalyst by filtration or centrifugation and analyzed by means of UV-Vis spectroscopy or HPLC. Controls will be conducted in order to differentiate photocatalytic degradation from other forms of pollutant removal.

IV. Structural Modification and Photocatalytic Properties of TiO_2-Based Nanocomposites

Photocatalytic activity in TiO_2-based nanocomposites is significantly influenced by the structural, morphological, and electronic features of the nanomaterials. Undoped TiO_2 typically shows good chemical stability and desirable photocatalytic properties, though its low activity under visible light limits the use of the vast majority of the solar spectrum. Formation of nanocomposites makes it possible to change the properties by incorporating appropriate secondary materials to change electronic properties and interfacial charge transfers. Coupling of semiconductors is one of the ways to increase photocatalytic activity. When two appropriate semiconductors with proper electronic structure are coupled, their interface can contribute to charge-carrier separation and decrease recombination processes. Type-II and Z-Scheme systems are just two examples of heterojunction mechanisms that can be obtained based on specific band alignments. It is essential, however, to identify the specific mechanism used.

Carbon-containing materials can offer extra benefits in terms of electron transfer, pollutant adsorption, and surface interactions. On the same note, certain metal and non-metal doping can affect the optical absorption and electronic behavior of such nanomaterials. Nevertheless, an overdose of modification can lead to the inhibition of active sites and/or formation of unwanted recombination routes, as well as reduce the stability of the catalyst itself. Characterization of such materials is thus necessary in order to comprehend their behavior. XRD is used to determine the crystal phase, while SEM and TEM can be used to assess the morphology and dispersion of the particles. FTIR and XPS can be used to determine the bonding and surface chemistry of the material. UV-Visible diffuse reflectance spectroscopy helps understand the optical absorption, while photoluminescence gives supporting data about the charge carrier recombination.

Visible-Light-Driven Degradation Mechanism of Emerging Organic Contaminants

Photocatalytic degradation using visible light involves light absorption, charge generation, charge separation, and surface oxidation–reduction reactions. Upon the absorption of the appropriate visible light photons by the modified TiO2 nanocomposite, electrons can become excited into high-energy electronic states resulting in positive holes. The charge carriers can move to the surface of the photocatalyst where they can react chemically with oxygen, water, and hydroxyl ions absorbed from solution. The electrons can reduce dissolved oxygen to produce superoxide-related reactive species if their reduction potentials are favorable. On the other hand, the photogenerated holes can oxidize adsorbed organic compounds or hydroxyl radicals if their energies allow. The reactive species can break down molecular bonds to transform pharmaceuticals, pesticides, dyes, and other organic contaminants into intermediate compounds. The degradation mechanism is dependent upon the electronic structure of the material, surface chemistry, pollutant nature, and reaction conditions. Solution pH can affect surface charges and pollutant adsorption, catalyst dose influences active sites and light absorption, whereas initial pollutant concentration can affect the apparent degradation rate due to competitive adsorption.

The efficiency of photocatalysis cannot be assessed just from the removal of the initial contaminant. There may be some intermediate compounds present in the solution, and the complete mineralization process may need more oxidation steps. Hence, the use of chromatographic analysis and the measurement of total organic carbon are vital when studying the degradation route and the mineralization capability. Also, radical scavenger tests may give information on which species are the main reactive agents. Catalytic activity in multiple cycles is essential when assessing catalysts' recyclability.

V. Results and Discussion

The proposed research is anticipated to show that proper modification of TiO2 would lead to an improvement in the performance of visible-light driven photocatalysis. Characterization would give insight into how the properties of the crystal structure, surface morphology and light absorption change after the formation of the nanocomposites. Reduction in photoluminescence intensity would suggest efficient charge separation, although other tests would be needed to elucidate charge transfer processes. Photocatalytic studies are expected to show that there is a difference in the ability of both pristine TiO2 and modified TiO2 to degrade contaminants. Better degradation performance might arise as a result of better visible-light absorption, surface affinity and production of reactive species. However, this will depend on the composition, dose, pollutant concentration and pH of the solution. Kinetics studies would show the apparent rate of reactions, while TOC tests would reveal mineralization levels. Cycle tests would reveal catalyst stability and reusability.

Comparative Analysis

Table 2 illustrates a qualitative comparison of pristine TiO_2 with modified TiO_2 nanocomposites based on significant factors considered for photocatalytic evaluation. These include possible benefits that nanocomposite modification can bring in terms of visible light absorption, carrier generation, surface characteristics, and pollutant removal. Performance improvement is not assured, however, as it would depend on the material composition, preparation process, and interface compatibility.

Table 2: Comparison of Pristine TiO_2 and Modified TiO_2-based Nanocomposites

Evaluation parameter	Pristine TiO_2	Modified TiO_2 nanocomposite
Light absorption	Primarily UV response	Potentially extended visible response
Charge separation	Recombination limitations	Potentially improved separation
Surface properties	Depends on synthesis	Tunable through modification
Pollutant adsorption	Material-dependent	Potentially enhanced
Photocatalytic activity	Limited under visible light	Expected improvement
Reusability	Generally stable material	Depends on composite stability

Graphical Evaluation

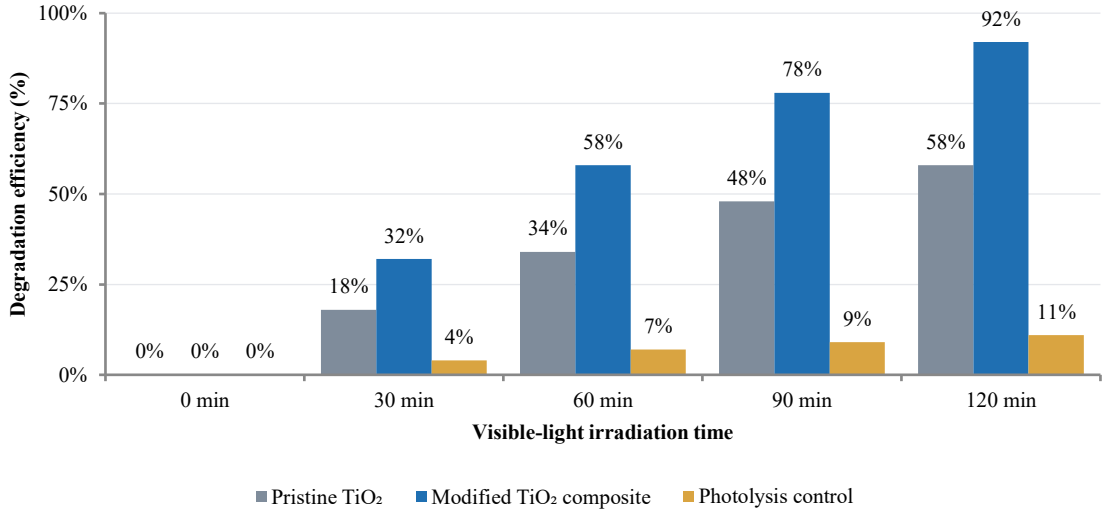


Figure 2: Illustrative Visible-Light Photocatalytic Degradation Efficiency over Irradiation Time

Figure 2 is a representation of the assumed correlation between time of exposure to light and the efficiency of organic pollutants removal by pristine TiO_2, TiO_2 nanocomposites modified, and photolysis controls. The assumed trend demonstrates increased degradation with increase in the duration of exposure, with a possibly higher rate for the modified composite. These are not actual experimental results that need to be substituted with actual measurements.

Discussion

The designed TiO_2 nanocomposites are anticipated to have enhanced photocatalytic behavior when exposed to visible light when compared to pristine TiO_2. Techniques such as XRD, SEM, TEM, and UV–Vis spectrophotometry can be used to investigate the crystallinity, surface morphology, particle distribution, and light absorption. Visible light absorption and lower electron-hole recombination can result in better production of reactive oxygen species, which can facilitate contamination degradation. Photocatalytic behavior will be assessed through degradation efficiency tests in relation to various irradiation periods, catalyst doses, pollutant concentration, and pH. The pseudo-first-order kinetics can be used to analyze the reaction rate for various catalyst compositions. Mineralization efficiency can be measured using total organic carbon determination.

Future Recommendations

1. Development of advanced nanocomposites: Explore new possibilities for semiconductor combinations, carbon-based compounds, and suitable dopants to enhance the efficiency of visible light absorption.
2. Solar light utilization: Perform experiments of photocatalysis under solar light as opposed to laboratory visible light sources.
3. Actual wastewater testing: Test the activity of photocatalyst on actual wastewater samples with various pharmaceuticals, pesticides, and organic pollutants.
4. Degradation path determination: Identify intermediate products using HPLC/LC–MS and determine possible degradation pathways.
5. Catalyst durability assessment: Repeat the photocatalysis cycle multiple times to test catalyst's recovery ability and durability.
6. Environmental safety concerns: Determine potential toxicity of degradation intermediates and nanoparticle release to the aqueous phase.
7. Feasibility study: Perform economic analysis of the synthesis cost, catalyst recycling needs, and energy consumption.

Challenges and Limitations

1. Limited visible light use: Some TiO2 modifications may lack adequate absorption or efficient separation of charges under practical lighting conditions.
2. Charge carriers recombination: The electron-hole recombination may decrease the amount of reactive agents needed to oxidize the pollutants.
3. Stability of nanocomposites: Some secondary materials may separate, decompose, or change their structure during the photocatalysis cycle.
4. Specific composition of wastewater: Salts, natural organic matter, and other pollutants present in wastewater can hinder photocatalytic reaction.
5. Medium toxicity: Partial decomposition may lead to creation of intermediates that will need further treatment.
6. Catalyst regeneration: It may be hard to recover fine particles from the treated water and will raise operational cost.
7. Laboratory vs. Field conditions: The lab results may not necessarily reflect the performance under natural sunlight conditions and actual wastewater.

VI. Conclusion

The objectives of this research are to synthesize and characterize the properties of TiO_2-based nanocomposites for the degradation of emerging organic contaminants via visible light irradiation. This research aims to overcome the limitations of traditional TiO_2 photocatalysts, namely limited absorption in the visible region and fast electron-hole recombination rates that affect its photocatalytic efficiency. The novelty in the research is the combination of nanocomposite preparation, detailed physical and chemical characterization, and photocatalytic study to correlate the properties of the prepared materials with their ability to degrade the organic contaminants. The proposed research includes the synthesis of modified TiO_2 nanocomposites and

analysis of the structural, morphological, chemical, and optical properties of the samples by means of XRD, SEM, TEM, FTIR, UV-Visible diffuse reflectance spectroscopy, photoluminescence, and BET analysis. The photocatalytic study of the samples will be done in the visible light and with selected emerging organic contaminants. According to expected outcomes, properly formulated TiO_2 nanocomposites might show better use of visible light, separation of carriers, and photocatalytic degradation efficiency compared to TiO_2 itself. This might lead to better elimination of persistent organic pollutants. However, the actual effectiveness will be contingent upon the composition of the nanocomposites, conditions of synthesis, properties of the pollutants, and process parameters. Experimentation will have to be performed in order to confirm the expected outcomes. Thus, the proposed research might provide a valuable scientific basis for creating photocatalytic materials suitable for wastewater purification. By establishing connections between material characteristics and degradation activity, this research might facilitate the creation of efficient, reusable, and eco-friendly TiO_2 photocatalytic systems in the future.

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