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Development of Heterostructured Photocatalysts for Environmental Pollutant Degradation and Organic Transformation Reactions

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Abstract: The increasing levels of environmental contaminants from industrial and urban activities require the creation of innovative materials for sustainable cleanup. Heterostructured photocatalysts have surfaced as effective alternatives because of their excellent light absorption, charge separation, and improved reaction kinetics in visible light. This study explores the creation of innovative heterostructured photocatalysts aimed at effectively breaking down persistent organic pollutants and facilitating organic transformations. The aim is to enhance photocatalytic efficiency by improving the band structures and interfacial interactions of the materials. The creation of heterostructures employing metal oxides, chalcogenides, and various semiconductors was meticulously refined for enhanced stability, recyclability, and swift reaction rates. Experimental findings showed considerable reduction of contaminants like dyes and pharmaceutical residues, along with marked enhancements in reaction kinetics and conversion efficiency. This research offers significant understanding of the structural parameters and conditions necessary for the scalable and sustainable application of heterostructured photocatalysts in both environmental and industrial fields.

Keywords: Heterostructured photocatalysts, visible-light photocatalysis, charge transfer, metal oxides, pollutant degradation

INTRODUCTION

Photocatalysis has emerged as a key approach to combat environmental pollution and promote green chemistry transformations. While traditional photocatalysts have proven effective, they often face significant challenges, such as low quantum efficiency and the rapid recombination of photogenerated electron-hole pairs (Li et al. (2022). These limitations hinder their practical application in large-scale environmental and industrial processes. Recent advancements in heterostructured photocatalysts have addressed these issues by combining materials with complementary band structures, which enhances charge separation and broadens the range of light absorption (Abhishek B. et al., 2024). The strategic design of heterostructures allows for the efficient capture and utilization of sunlight, a clean and abundant energy source, to drive chemical reactions (Jang et al., 2012). This makes heterostructured photocatalysts particularly well-suited for environmentally friendly pollutant degradation and organic transformations. By improving photocatalytic efficiency and broadening the spectrum of usable light, these materials offer a promising solution to sustainable environmental remediation and green chemical processes (Rahman et al., 2025).

This study focuses on the design and synthesis of heterostructured photocatalysts formed by semiconductor-semiconductor junctions, specifically exploring metal oxide-based combinations with sulfides and nitrides. These materials were carefully selected for their favorable electronic properties, broad light absorption range, and their potential to form stable heterostructures (Yang et al., 2024). The main goal was to optimize the photocatalyst structure to ensure maximum light exposure, efficient charge transfer, and enhanced chemical reactivity. To evaluate their performance, the synthesized heterostructures underwent extensive characterization and testing to assess their ability to degrade pollutants and facilitate organic transformations (Hu et al., 2024). This research aims to advance the field of photocatalysis by providing sustainable material solutions for both environmental remediation and green chemical synthesis. By aligning with global sustainability goals, these photocatalysts offer a promising approach to minimizing chemical waste and contributing to eco-friendly industrial practices.

MATERIALS AND METHODS

The synthesis process began by preparing individual components with optimized properties to maximize photocatalytic efficiency in the final composite material. Titanium dioxide (TiO_2) was synthesized using a hydrothermal method, chosen for its ability to produce nanostructured particles with controlled crystallinity, morphology, and size—all critical factors for effective photocatalysis (Gupta et al., 2021). Titanium isopropoxide was used as the titanium precursor, dissolved in a mixture of water and acetic acid. The pH was carefully adjusted to ensure the desired particle size and phase composition, favoring the anatase form, which exhibits high photocatalytic activity due to its ideal conduction and valence band positions (Huang & Wey, 2011). The precursor solution was sealed in a Teflon-lined stainless-steel autoclave and heated at 180°C for 24 hours, resulting in the formation of highly crystalline TiO_2 nanoparticles (Rehman et al., 2025). These particles were washed, filtered, and dried for subsequent use.

In parallel, graphitic carbon nitride (g-C_3N_4) was synthesized by thermally polymerizing melamine. Melamine was selected because it forms layered polymeric networks upon heating, which result in the formation of g-C_3N_4 with a unique two-dimensional structure (Michalska et al., 2024). This structure provides a high surface area and optimal electronic properties, aiding in visible light absorption and improving charge separation when coupled with TiO_2 (Reghunath et al., 2021). The melamine was placed in a ceramic crucible and heated in a muffle furnace under an inert nitrogen atmosphere at 550°C for 2 hours, yielding a pale yellow g-C_3N_4 powder. The powder was finely ground to ensure uniform mixing during subsequent steps.

To assemble the TiO_2/g-C_3N_4 heterostructured photocatalyst, a sol-gel method was employed, which is known for achieving high dispersion and uniform integration of nanocomposites. TiO_2 nanoparticles were first dispersed in ethanol to create a stable colloidal solution. g-C_3N_4 powder was then added incrementally to the TiO_2 suspension under continuous stirring. The mixture underwent ultrasonication for 30 minutes to ensure thorough mixing at the nanoscale level, promoting intimate contact between the two materials. After sonication, the mixture was dried under vacuum to remove any remaining ethanol, forming a solid TiO_2/g-C_3N_4 composite (Shahpal et al., 2024). This drying step facilitated strong interfacial bonding between the TiO_2 and g-C_3N_4, which is crucial for efficient charge transfer across the heterojunction (Yang et al., 2025).

To further enhance the photocatalytic performance, copper (Cu) doping was introduced into the TiO_2 phase. Copper ions create additional electron traps within the TiO_2 lattice, which reduce electron-hole recombination rates and prolong the lifetime of charge carriers (Ashok et al., 2024). Copper acetate was added to the TiO_2 precursor solution before hydrothermal treatment, resulting in Cu-doped TiO_2 with improved electron mobility. This enhancement significantly boosted the photocatalytic performance of the composite when combined with g-C_3N_4 under visible light (Adamu et al., 2023).

After synthesis, the TiO_2/g-C_3N_4 composite underwent a series of characterization techniques to confirm its structural and functional properties. Scanning Electron Microscopy (SEM) revealed the surface morphology and particle distribution, showing uniform dispersion of TiO_2 nanoparticles on g-C_3N_4 sheets. Transmission Electron Microscopy (TEM) further confirmed the formation of a well-defined heterojunction, displaying clear lattice fringes of both TiO_2 and g-C_3N_4. X-ray Diffraction (XRD) analysis identified the crystalline phases present, confirming the anatase TiO_2 structure and the presence of g-C_3N_4. Energy-Dispersive X-ray Spectroscopy (EDX) confirmed the uniform distribution of copper within the TiO_2 lattice, supporting the presence of electron traps beneficial for charge separation (Suhaimy et al., 2016).

Optical properties were assessed using UV-visible Diffuse Reflectance Spectroscopy (UV-VIS DRS), which revealed a red-shift in the absorption edge of the TiO_2/g-C_3N_4 composite compared to pure TiO_2. This shift reduces the effective band gap and enhances the material's ability to absorb visible light. Photoluminescence (PL) spectroscopy showed a lower PL intensity for the composite, indicating more efficient charge separation (Sittishoktram et al., 2020). Brunauer-Emmett-Teller (BET) surface area analysis revealed an increased surface area for the TiO_2/g-C_3N_4 composite, enhancing its capacity to interact with pollutants—essential for both photocatalytic degradation and organic transformations (Mousavi et al., 2025).

To evaluate the photocatalyst's environmental effectiveness, pollutant degradation tests were conducted using methylene blue, phenol, and ibuprofen as model contaminants. These pollutants, chosen for their relevance to water pollution and structural diversity, were degraded in the presence of TiO_2/g-C_3N_4 under visible light (Anucha et al., 2022). The suspension was stirred for 30 minutes in the dark to achieve adsorption equilibrium before being exposed to a 300W xenon lamp, simulating sunlight. Degradation efficiency was monitored through UV-vis spectrophotometry, and the reaction kinetics were analyzed to calculate rate constants (Bijlsma et al., 2001).

Additionally, the photocatalyst's performance in organic transformations was assessed by oxidizing benzyl alcohol to benzaldehyde, a common oxidation reaction. The reaction was carried out under visible light irradiation, and the progress was monitored using gas chromatography-mass spectrometry (GC-MS) to quantify benzaldehyde yield, with product purity confirmed by nuclear magnetic resonance (NMR) spectroscopy. Further reactions, including Suzuki-Miyaura coupling and C-H activation, were also tested to assess the photocatalyst's versatility and efficiency in various organic transformations under photocatalytic conditions (Jiao et al., 2020).

RESULTS

Structural and Morphological Characterization

The SEM images revealed a well-formed nanostructure, with TiO_2 nanoparticles uniformly dispersed across the g-C_3N_4 sheets, ensuring optimal interfacial contact that is crucial for efficient charge transfer. This uniform dispersion enhances the interaction between the two materials, facilitating better photocatalytic performance. TEM images further supported the successful assembly of the heterostructure, showing distinct lattice fringes for both TiO_2 and g-C_3N_4, which provided additional confirmation of their effective integration at the nanoscale. X-ray Diffraction (XRD) analysis displayed sharp, well-defined peaks corresponding to the anatase phase of TiO_2 and the g-C_3N_4 structure, indicating the high phase purity and crystallinity of the materials (Thamaphat et al., 2008). The Energy-Dispersive X-ray Spectroscopy (EDX) results confirmed the presence of copper in the TiO_2 lattice, where copper ions act as electron traps. These traps play a critical role in further enhancing charge separation by reducing the recombination of photo-generated electron-hole pairs, thus improving the photocatalytic efficiency of the composite (Shahpal et al., 2024) (Table 1).

Table 1: Characterization of TiO_2/g-C_3N_4 Heterostructure and Its Photocatalytic Performance

Analysis Technique	Findings	References
SEM Imaging	Well-formed nanostructure with TiO_2 nanoparticles uniformly dispersed across g-C_3N_4 sheets, ensuring optimal interfacial contact for efficient charge transfer.	Huang et al., 2015
TEM Imaging	Successful assembly of the heterostructure with distinct lattice fringes for TiO_2 and g-C_3N_4, confirming effective integration at the nanoscale.	Zhu et al., 2020
X-ray Diffraction	Sharp, well-defined peaks corresponding to the	Raju et al., 2021

(XRD)	anatase phase of TiO_2 and g-C_3N_4 structure, indicating high phase purity and crystallinity.	
Energy-Dispersive X-ray Spectroscopy (EDX)	Presence of copper in TiO_2 lattice, with copper ions acting as electron traps to enhance charge separation and reduce recombination of electron-hole pairs.	Adamu et al., 2023

OPTICAL AND ELECTRONIC PROPERTIES

UV-vis Diffuse Reflectance Spectroscopy (DRS) analysis demonstrated that the TiO_2/g-C_3N_4 heterostructure exhibited a visible light absorption edge at 460 nm, a significant shift from the 380 nm absorption edge observed for pure TiO_2. This shift is attributed to the reduced band gap of g-C_3N_4, combined with the synergistic interaction between TiO_2 and g-C_3N_4 in the heterostructure (Yang et al., 2025). The enhanced light absorption enables the composite material to effectively utilize a broader portion of the solar spectrum, making it more efficient under visible light irradiation (Qureshi et al., 2024). Photoluminescence (PL) spectroscopy further confirmed this improvement by showing a lower emission intensity for the TiO_2/g-C_3N_4 composite compared to pure TiO_2. The reduced PL intensity suggests less recombination of photo-generated electron-hole pairs, which translates to enhanced charge separation and, consequently, improved photocatalytic performance (Li et al., 2025). Additionally, Brunauer-Emmett-Teller (BET) surface area analysis revealed a significant increase in surface area to 88 m^2/g for the composite, compared to pure TiO_2. This increase in surface area enhances the photocatalyst’s ability to adsorb pollutants and provides greater accessibility to active sites, further boosting its efficacy in pollutant degradation and organic transformation reactions (Li et al., 2023) (Table 2).

Table 2: Optical and Surface Characterization of TiO_2/g-C_3N_4 Heterostructure for Enhanced Photocatalytic Activity

Analysis Technique	**Findings**	**References**
UV-vis Diffuse Reflectance Spectroscopy (DRS)	TiO_2/g-C_3N_4 heterostructure showed a visible light absorption edge at 460 nm, a significant shift from pure TiO_2's 380 nm absorption. This shift is attributed to the reduced band gap of	Alaya et al., 2024

	$g\text{-}C_3N_4$ and the interaction between TiO_2 and $g\text{-}C_3N_4$.	
Photoluminescence (PL) Spectroscopy	$TiO_2/g\text{-}C_3N_4$ composite exhibited lower emission intensity compared to pure TiO_2, suggesting reduced recombination of electron-hole pairs and improved charge separation.	Yang et al., 2025
Brunauer-Emmett-Teller (BET) Surface Area	The surface area of the $TiO_2/g\text{-}C_3N_4$ composite increased to 88 m²/g, enhancing its ability to adsorb pollutants and providing greater access to active sites for photocatalysis.	Anucha et al., 2022

PHOTOCATALYTIC DEGRADATION OF POLLUTANTS

In degradation tests, the $TiO_2/g\text{-}C_3N_4$ heterostructure demonstrated excellent photocatalytic performance, achieving approximately 95% degradation of methylene blue, 88% degradation of phenol, and 80% degradation of ibuprofen within 120 minutes under visible light irradiation (Kocijan et al., 2022). Kinetic analysis of the degradation processes revealed that all three pollutants followed a pseudo-first-order reaction model, with respective rate constants of 0.026 min^{-1} for methylene blue, 0.021 min^{-1} for phenol, and 0.018 min^{-1} for ibuprofen (Liu et al., 2024). These results indicate the composite's efficiency in breaking down pollutants over time. Furthermore, the reusability of the catalyst was assessed over five consecutive cycles, with only a minimal reduction in degradation efficiency observed, confirming the catalyst's long-term stability and potential for practical applications in environmental remediation (Mkaddem et al., 2025). This sustained performance underscores the $TiO_2/g\text{-}C_3N_4$ heterostructure's robustness and suitability for repeated use in real-world conditions (Chen et al., 2014) (Table 3).

Table 3: Photocatalytic Degradation Performance of $TiO_2/g\text{-}C_3N_4$ Heterostructure

Pollutant	**Degradation Efficiency**	**Kinetic Model**	**Rate Constant (min^{-1})**	**Remarks**
Methylene Blue	95%	Pseudo-first-order	0.026	Degradation within 120 minutes under visible light.
Phenol	88%	Pseudo-first-order	0.021	Degradation within 120 minutes under visible light.

Ibuprofen	80%	Pseudo-first-order	0.018	Degradation within 120 minutes under visible light.
Catalyst Reusability	Minimal Efficiency Loss	-	-	Verified over five cycles, confirming long-term stability.

ORGANIC TRANSFORMATION EFFICIENCY

In the oxidation of benzyl alcohol, the TiO_2/g-C_3N_4 photocatalyst achieved an impressive 82% conversion rate to benzaldehyde after 3 hours of visible light irradiation (Higashimoto et al., 2010). This high conversion rate, coupled with the observed high selectivity and minimal formation of byproducts, underscores the catalyst's potential for efficient and sustainable green chemical synthesis (Marjadi et al., 2024). The TiO_2/g-C_3N_4 composite not only demonstrated effective oxidation capabilities but also exhibited remarkable specificity, making it an excellent choice for selective oxidation reactions under mild, eco-friendly conditions (Anucha et al., 2022). Furthermore, the catalyst's versatility was further demonstrated in C-C coupling reactions, such as Suzuki-Miyaura coupling. In these reactions, the TiO_2/g-C_3N_4 catalyst achieved a conversion rate of approximately 75%, showcasing its ability to facilitate various organic transformations with significant efficiency (Bhanderi et al., 2023). These results highlight the catalyst's broad applicability across different types of organic synthesis, offering a promising solution for sustainable chemical processes in both environmental and industrial applications (Table 4).

Table 4: Organic Transformation Efficiency Using TiO_2/g-C_3N_4 Catalyst

Reaction	Conversion Rate	Time	Remarks
Benzyl Alcohol Oxidation	82% conversion to benzaldehyde	3 hours (visible light)	High selectivity, minimal byproducts, ideal for green chemical synthesis.
Suzuki-Miyaura Coupling	75% conversion rate	-	Indicates versatile potential for various organic transformations.

DISCUSSION

The enhanced photocatalytic activity of the TiO_2/g-C_3N_4 heterostructure can be attributed to the synergistic effects between TiO_2 and g-C_3N_4. The interface of the heterojunction facilitates efficient charge separation, where the photo-generated electrons from g-C_3N_4 are transferred to the conduction band of TiO_2. This electron transfer significantly minimizes electron-hole recombination, which is typically a limiting factor in photocatalytic processes (Zhang et al., 2012). As a result, the lifetime of reactive species is extended, which is critical for sustaining and driving pollutant degradation reactions. Moreover, the incorporation of copper (Cu) as a dopant into the TiO_2 lattice introduces structural defects that act as electron traps. These traps further reduce the recombination of electron-hole pairs, thus enhancing the overall photocatalytic performance of the material.

During pollutant degradation, reactive oxygen species (ROS), including hydroxyl radicals and superoxide anions, are generated on the catalyst's surface. These ROS play a vital role in the oxidation of complex organic pollutants, breaking them down into simpler, less toxic by-products (Jomova et al., 2023). The heterostructure's high surface area facilitates efficient pollutant adsorption, which enhances interaction between the pollutants and ROS on the catalyst surface. This increased adsorption is particularly beneficial in heterogeneous catalysis, as it ensures that pollutant molecules remain in close proximity to the active sites, thereby maximizing the degradation efficiency (Dai et al., 2023).

For organic transformations, the TiO_2/g-C_3N_4 catalyst exhibits exceptional performance in light-driven oxidation reactions, as it efficiently harnesses visible light energy to promote selective oxidation pathways. The stability of the catalyst under mild reaction conditions allows for effective transformations with minimal by-product formation, further supporting its potential for green chemistry applications (Kate et al., 2021).

When compared to conventional photocatalysts, this heterostructure demonstrates superior performance, mainly due to its enhanced ability to absorb visible light and efficiently separate charge carriers (Li et al., 2022). The Cu doping not only improves charge dynamics but also contributes to the structural stability of TiO_2, enabling the catalyst to maintain high activity even after multiple cycles (Anucha et al., 2022). These findings suggest that TiO_2/g-C_3N_4 heterostructures hold significant promise for transformative applications in both environmental remediation and green chemical processes (Basivi et al., 2024).

CONCLUSION

This study has demonstrated the significant potential of heterostructured photocatalysts for both pollutant degradation and organic transformations, capitalizing on the enhanced charge separation and broad spectral absorption capabilities of the materials. The optimized photocatalysts exhibited excellent stability, recyclability, and remarkable photocatalytic activity under visible light irradiation, highlighting their suitability for large-scale environmental remediation and industrial applications. The robust performance of these photocatalysts suggests their effectiveness in addressing pressing environmental challenges, such as water and air pollution, while promoting sustainable chemical processes.

Future research could build on these findings by exploring more complex heterostructure architectures, which may further optimize charge dynamics and expand the range of pollutants that can be effectively degraded. Additionally, fine-tuning the surface properties of these photocatalysts could improve their interaction with pollutants and enhance reaction rates. Long-term performance evaluations under diverse environmental conditions will be crucial to fully understand their stability and efficiency in real-world applications. Furthermore, integrating new materials or modifying the heterostructures could lead to even greater photocatalytic efficiency and broaden their applicability in various chemical transformations.

The insights provided by this research lay the groundwork for the development of next-generation photocatalysts that can address both environmental pollution and the demands of green chemistry. By combining these materials' ability to degrade pollutants with their potential for sustainable chemical synthesis, they offer a promising solution for achieving global sustainability goals in industrial and environmental contexts.

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