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Research Progress and Reaction Mechanisms of Different Types of Photocatalysts

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Abstract. Solar energy, as a critical clean energy source, holds significant importance for addressing energy and environmental challenges. Photocatalytic technology utilizes sunlight to drive chemical reactions, enabling not only pollutant degradation (e.g., wastewater purification) but also the conversion of carbon dioxide into organic fuels (such as methane and methanol), while facilitating energy storage. This dual value positions it as a vital solution for both environmental governance and energy security. This review systematically examines the mechanisms and applications of photocatalytic technology, with a focus on four catalyst categories: metal oxides (e.g., WO_3), which enhance visible-light response by optimizing band structures; metal sulfides (e.g., ZnS), which leverage narrow bandgaps to improve light absorption but require solutions to mitigate photocorrosion; non-metallic compounds (e.g., graphitic carbon nitride, g-C_3N_4), which serve as cost-effective materials where doping or defect engineering boosts carrier separation efficiency; and metal-organic frameworks (MOFs), which exploit high porosity and tunable structures to achieve efficient substrate adsorption and catalytic site design. The spatial separation of photogenerated electron-hole pairs within the heterojunction structure effectively suppresses charge carrier recombination, thereby enhancing quantum efficiency. Although photocatalytic technology has achieved significant breakthroughs in pollutant degradation and clean energy production, it still faces several challenges. These include low energy conversion efficiency, unstable catalyst performance, and high costs associated with large-scale applications.

Keywords: Photocatalyst, Heterojunction, Photocatalytic reactions.

1. Introduction

Amid worsening global environmental conditions, humanity is actively exploring diverse clean energy sources, with solar energy standing out as a critically important option. Photocatalytic technology enables direct utilization of solar energy to drive redox reactions. It effectively breaks down pollutants while minimizing secondary pollution during the decomposition process, thereby achieving highly efficient wastewater treatment [1].

Beyond wastewater treatment, this photocatalytic material can also utilize its unique physical and chemical properties to convert carbon dioxide into chemical fuels such as carbon monoxide and methane [2], demonstrating considerable potential in enhancing energy security. In practical daily

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applications, photocatalytic nanocomposites can be coated onto fabrics and automotive glass surfaces to achieve self-cleaning functionality, significantly reducing maintenance costs.

Semiconductors dominate photocatalytic materials due to band structures that enhance charge separation and extend carrier lifetimes. However, non-semiconductor materials like metal complexes can achieve similar functions through electron-transfer pathways.

This paper focuses on photocatalytic reactions and photocatalysts, aiming to summarize the characteristics and performance of different types of photocatalysts and explore their applications. It will review several common photocatalysts, present their key characteristics, and propose suggestions for future development in photocatalytic research.

2. Photocatalytic mechanism

Photocatalytic reactions (Fig.1) proceed by exciting electrons in catalysts with suitable band structures (e.g., semiconductors like TiO_2 or g-C_3N_4), driving electron transitions from the valence band (VB) to the conduction band (CB) to form electron-hole pairs. The holes (h^+) in the VB exhibit strong oxidizing properties, reacting with water molecules (H_2O) or surface-adsorbed hydroxide ions (OH^-) to generate highly reactive hydroxyl radicals (•OH). Simultaneously, electrons (e^-) in the CB reduce oxygen (O_2) to form superoxide radicals (•O_2^-). In aqueous solutions, •OH preferentially oxidizes organic pollutants through reactions such as hydrogen atom abstraction or addition to unsaturated bonds. Meanwhile, •O_2^- further transforms into hydrogen peroxide (H_2O_2), which decomposes to yield additional •OH radicals. This reaction achieves the degradation and mineralization of organic compounds, converting them into CO_2, H_2O, and inorganic ions [3].

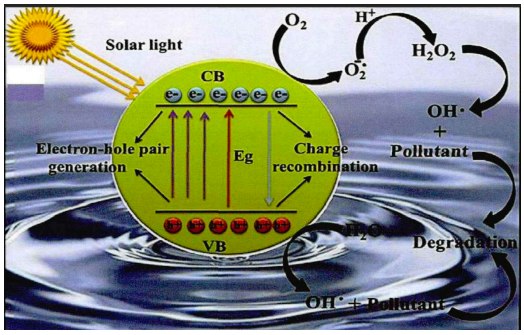


Figure 1. Photocatalytic process [3]

3. Types of photocatalysts

3.1. Metal oxide semiconductors

3.1.1. Introduction to metal oxide semiconductors

Metal oxide semiconductors consist of metal and oxygen elements, exhibiting semiconductor properties alongside exceptional chemical stability, thermal stability, high electron mobility, tunable characteristics, and cost-effectiveness. These metal oxide semiconductors are similarly classified into n-type and p-type semiconductors. n-type semiconductors include tin oxide, titanium dioxide, zinc oxide, and tungsten trioxide, while typical p-type semiconductors include cuprous oxide. These metal oxides possess distinct physical and chemical properties, making them widely applicable in electronics, electrical devices, and sensors. They play critical roles not only in photocatalytic reactions but also in electronic components and sensor technologies.

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3.1.2. Properties and applications of tungsten trioxide (WO3) semiconductor

Tungsten trioxide (WO_3) is a typical n-type semiconductor material with a bandgap ranging from 2.6 to 2.8 electron volts. This characteristic enables strong visible light absorption, resulting in high photocatalytic efficiency. Its valence band primarily consists of O 2p orbitals, while the conduction band is formed by W 5d orbitals. Under visible light irradiation, it generates reactive oxygen species through photogenerated electron-hole reactions, effectively degrading organic pollutants in wastewater and facilitating water purification [4].

Despite its broad applications in pollutant degradation, water splitting for oxygen evolution, CO_2 reduction, and photocatalytic sterilization, WO_3 faces limitations due to its relatively positive conduction band position, preventing standalone use in photocatalytic water splitting for hydrogen production. Instead, it functions effectively as a photoanode material paired with reduction catalysts in photoelectrochemical systems. To enhance its photocatalytic activity, strategies such as elemental doping (e.g., nitrogen to narrow the bandgap), morphology control (nanostructuring to increase surface area), surface decoration (e.g., noble metal loading to accelerate charge transfer), and heterojunction construction (e.g., WO_3/BiOCl for reduced carrier recombination) are employed. However, challenges like high carrier recombination rates and the inherent conduction band limitation necessitate further research into band engineering and interface design for practical applications.

3.2. Metal sulfide

3.2.1. Metal sulfide semiconductors overview

Metal sulfide semiconductors, comprising metal elements bonded with sulfur, have gained significant research attention due to their cost-effectiveness, environmental compatibility, high carrier mobility, and robust chemical stability. Classified into binary (e.g., ZnS, CdS, CuS), ternary (e.g., ZnCdS, CdSSe), and quaternary sulfides, these materials demonstrate versatile applications in photocatalytic water splitting, solar cells, gas sensing, lithium/sodium-ion batteries, and electrocatalysis. Binary sulfides exhibit structural simplicity and mature synthesis, with CdS serving as a window layer in photovoltaic devices, while MoS_2 contributes high theoretical capacity in energy storage systems, establishing their fundamental role in advancing sustainable technologies.

3.2.2. Characteristics and optimization of zinc sulfide (ZnS)

Zinc sulfide (ZnS), a representative binary sulfide semiconductor, encounters three primary limitations: its wide bandgap (3.6–4.8 eV) restricts light absorption to the ultraviolet spectrum (<5% of solar irradiance), elevating electron-hole recombination rates which diminish photocatalytic efficiency, and poor chemical stability leading to photocorrosion in aqueous environments. To overcome these constraints, strategic modifications are employed. Metal doping incorporates transition metals (e.g., Cu^{2+}) or rare-earth ions, creating intermediate energy levels that broaden light absorption while suppressing carrier recombination; rare-earth ions further enhance photon conversion through energy-level transitions. Alternatively, non-metal doping with nitrogen or carbon optimizes band structures: nitrogen atoms substituting sulfur generate N 2p-Zn 3d hybridization, introducing new energy levels near the valence band edge and narrowing the bandgap to ~2.8 eV, thereby enabling efficient visible-light-driven hydrogen production and pollutant degradation. Carbon atoms interstitially integrated improve electron mobility via C 2p orbital hybridization.

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Concurrent surface defect engineering (e.g., engineered sulfur vacancies) extends charge carrier lifetimes. Modified ZnS-based composites, such as ZnS/CuS heterojunctions, exhibit markedly enhanced performance in visible-light photocatalysis and sensing applications, indicating substantial potential for future sustainable technologies [5].

3.3. Non-metal photocatalysts

3.3.1. Overview of non-metal photocatalysts

Non-metal photocatalysts offer significant advantages over traditional metal-based materials, including lower production costs, scalability for mass production, and enhanced chemical stability and durability. These characteristics make them environmentally safer and more sustainable for practical applications. Represented by graphitic carbon nitride (g-C_3N_4), non-metal catalysts demonstrate broad potential in energy regeneration, environmental remediation, antimicrobial activity, sensing, electrochemical storage, and bioimaging. Their unique electronic structures and tunable band properties provide innovative pathways for efficient solar energy utilization, positioning them as pivotal materials for advancing green technologies.

3.3.2. Properties and optimization of graphitic carbon nitride (g-C_3N_4)

Graphitic carbon nitride (g-C_3N_4), a metal-free polymeric semiconductor, features a graphene-like layered structure composed of repeating C_3N_3 (triazine) and C_6N_7 (heptazine) units interconnected via sp^2 hybridization, forming an extensively delocalized π-conjugated system. The C_6N_7 units exhibit superior thermodynamic stability, endowing g-C_3N_4 with high chemical robustness and a narrow bandgap (~2.7 eV), enabling visible-light absorption (450–460 nm) and overcoming the spectral limitations of conventional photocatalysts. Synthesized from earth-abundant carbon and nitrogen precursors, g-C_3N_4 is cost-effective, non-toxic, and eco-friendly, addressing the high costs and heavy-metal contamination associated with metal oxide catalysts [6].

However, unmodified g-C_3N_4 suffers from inherent limitations: low surface area, scarce active sites, and rapid recombination of photogenerated carriers. To enhance performance, strategies such as elemental doping (e.g., sulfur or nitrogen to modulate band structures) and heterojunction construction (e.g., coupling with metal oxides or carbon materials) are employed. Introducing microporous architectures increases surface area and active sites, while decorating with noble metal nanoparticles (e.g., Pt) or carbon quantum dots suppresses charge recombination. Further optimizations via morphological engineering (e.g., ultrathin nanosheets) and surface functionalization (e.g., edge-oxidation) significantly improve charge separation efficiency and light-harvesting capabilities, unlocking practical applications in pollutant degradation and photocatalytic hydrogen evolution [7].

3.4. Metal-Organic Frameworks (MOFs)

3.4.1. Characteristics and challenges of Metal-Organic Frameworks (MOFs) in photocatalysis

Metal-organic frameworks (MOFs), formed by the self-assembly of metal nodes and organic ligands, are porous crystalline materials characterized by ultra-high porosity (greater than 90%), exceptionally large specific surface area, and tunable structure and composition, which collectively underpin their significant potential in photocatalysis. In practical applications, MOFs fulfill three primary roles: as photocatalysts, they directly absorb light energy to generate electron-hole pairs,

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serving as the primary agents for converting solar energy into chemical energy; as co-catalysts, they optimize interfacial charge transfer pathways to promote carrier separation, thereby enhancing overall catalytic reaction efficiency; and as host materials, they provide carriers for active components, leveraging their structural properties to support catalytic activity even when their inherent catalytic capability is limited, often requiring integration into composite systems for optimal functionality.

3.4.2. Limitations of Metal-Organic Frameworks (MOFs) in photocatalysis

As emerging materials with ultra-high porosity (greater than 90%), large specific surface area, and structural tunability, MOFs exhibit promise in applications such as photocatalytic water splitting and CO_2 reduction. However, their practical implementation faces three key limitations: Applicability constraints restrict stable catalytic activity to only a few MOFs (e.g., zirconium/iron-based systems), while most materials fail to meet requirements due to band mismatch or high carrier recombination rates. Insufficient catalytic activity results in hydrogen production or CO_2 conversion efficiencies far below industrial demands, necessitating structural engineering or heterojunction composites for enhancement. Many photocatalysts rely heavily on precious metals such as platinum (Pt) and palladium (Pd), which significantly increase technology costs, thereby hindering their widespread adoption.Future research must focus on non-precious metal modification strategies and water stability optimization to advance the practical application of MOF-based photocatalytic technologies.

4. Heterojunctions

4.1. Advances and challenges in photocatalysts

Traditional photocatalysts face significant limitations despite their capability to produce hydrogen. Key drawbacks include challenges in catalyst recovery, poor structural stability, limited specific surface area, and high production costs. In contrast, two-dimensional (2D) material-based catalysts offer a transformative solution. Compared to bulk materials, 2D catalysts exhibit substantially higher specific surface areas, shorter charge carrier transport pathways, and broader light absorption ranges. These properties enable more efficient solar energy harvesting and utilization.

Furthermore, 2D materials maintain structural integrity under prolonged illumination, ensuring stable catalytic performance. While monolayer 2D materials may suffer from rapid photogenerated electron-hole recombination—which can compromise hydrogen evolution efficiency—researchers are actively addressing this issue through strategic modifications. Among these, heterojunction structures formed by stacking two distinct monolayers have proven particularly effective. Based on band alignment principles, heterojunctions are categorized into three types: Type-I, Type-II, and Type-III.

4.2. Band structure and carrier behavior in Type-I heterojunctions

The Type-I heterojunction (also known as a straddling-gap heterojunction) is formed by two distinct semiconductor materials (labeled A and B). Its defining feature is that the conduction band minimum (CBM) of semiconductor A lies below that of semiconductor B, while the valence band maximum (VBM) of semiconductor A is higher than that of semiconductor B (as illustrated in Fig. 2). This band alignment results in the complete envelopment of semiconductor B's conduction and valence bands within the energy band range of semiconductor A, forming a quantum-well-like structure.

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Under light excitation, photogenerated electrons transition from the conduction band of semiconductor B to the lower-energy conduction band of semiconductor A, while photogenerated holes migrate from the valence band of semiconductor B to the higher-energy valence band of semiconductor A. Consequently, both electrons and holes accumulate in semiconductor A, leading to ineffective spatial separation of the two types of charge carriers [8].

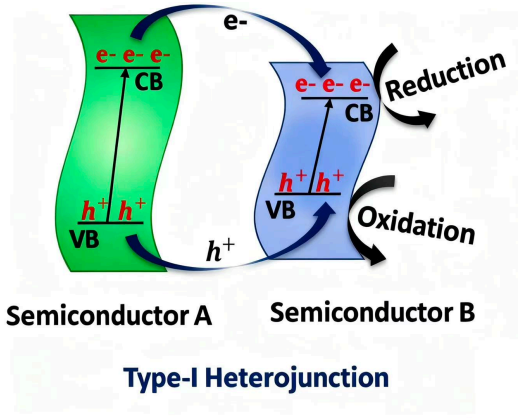


Figure 2. Mechanism of Type-I heterojunctions [8]

4.3. Type-II heterojunctions

4.3.1. Charge separation mechanism and limitations in Type-II heterojunctions

In Type-II heterojunctions (as illustrated in Fig. 3), the conduction band minimum (CBM_A) and valence band maximum (VBM_A) of semiconductor A are positioned higher than those of semiconductor B (CBM_B and VBM_B). Under light excitation, photogenerated electrons migrate from CBM_A to CBM_B, while holes transfer from VBM_B to VBM_A, achieving spatial separation of electron-hole pairs. However, this band alignment weakens the redox capability: reduction reactions occur on the conduction band of semiconductor B (where the higher CBM_B position results in lower reduction potential), while oxidation reactions proceed on the valence band of semiconductor A (where the lower VBM_A position leads to weaker oxidation potential), collectively diminishing the thermodynamic driving force for photocatalytic reactions.

Additionally, practical charge transfer faces kinetic barriers.Firstly repulsion between like charges (e.g., electrons in CBM_A and CBM_B, holes in VBM_A and VBM_B) impedes interfacial carrier migration.Secondly electrostatic attraction between electrons and holes further suppresses spatial charge separation efficiency.Consequently, electrons accumulate in CBM_B (weak reducibility) and holes in VBM_A (weak oxidizability), limiting photocatalytic activity. In contrast, Z-scheme heterojunctions (inspired by plant photosynthesis) utilize built-in electric fields to recombine carriers with weak redox capabilities (e.g., electrons in CBM_B and holes in VBM_A), while retaining strongly reducing electrons (in CBM_A) and oxidizing holes (in VBM_B), thereby synergizing effective charge separation with high redox activity.

4.3.2. Z-scheme heterojunction

The Z-scheme heterojunction is a specialized variant of the Type-II heterojunction structure, named for its characteristic "Z"-shaped electron transfer pathway in the energy band diagram. While its band alignment resembles that of a conventional Type-II heterojunction (where the conduction and

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valence bands of two semiconductors are staggered), its charge transfer mechanism differs significantly. Under visible light irradiation (Fig.3), electrons in both semiconductors are excited to their conduction bands (CB), while holes remain in their valence bands (VB). Crucially, in the Z-scheme system, photogenerated holes from the valence band of Semiconductor 1 (PS-I) migrate to the interface and recombine with photogenerated electrons from the conduction band of Semiconductor 2 (PS-II). This selective recombination preserves the high-energy photogenerated electrons in the conduction band of PS-I and the high-energy holes in the valence band of PS-II. Consequently, PS-I retains strongly reductive electrons, and PS-II retains strongly oxidative holes, achieving both efficient spatial separation of charge carriers and maximized redox potential. Compared to traditional Type-I (straddling gap) and Type-II (staggered gap) heterojunctions, the Z-scheme design not only optimizes carrier separation efficiency but also prevents the reduction in redox capability caused by charge migration to lower-energy band positions, making it particularly advantageous for applications like photocatalytic water splitting, CO_2 reduction, and pollutant degradation [9].

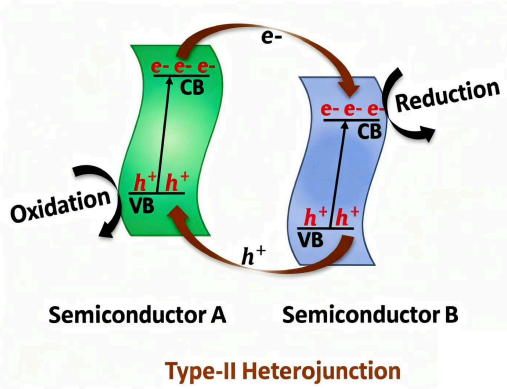


Figure 3. Mechanism of Type-II heterojunctions [8]

4.3.3. S-scheme heterojunction

In 2020, a research team innovatively proposed the concept of the S-scheme heterojunction based on the Z-scheme framework. Within this configuration, when two semiconductors come into contact, their Fermi levels realign to reach equilibrium, resulting in band bending deformation at the interface. This process generates a built-in electric field directed from the photocatalyst with stronger reducing capability toward the one with stronger oxidizing capability [10].

4.4. Charge transfer mechanism and limitations in Type-III heterojunctions

In Type-III heterojunctions (as illustrated in Fig. 4), the valence band maximum (VBM) of semiconductor A is positioned above the conduction band minimum (CBM) of semiconductor B, resulting in a staggered bandgap alignment where the energy bands of the two semiconductors exhibit no overlapping region. This band configuration prevents photogenerated electrons from migrating from the CBM of A to the CBM of B, while simultaneously blocking the transfer of photogenerated holes from the VBM of B to the VBM of A. Consequently, the interfacial carrier migration pathway is entirely disrupted. As a result, Type-III heterojunctions fail to achieve effective spatial separation of electron-hole pairs, rendering them incapable of enhancing photocatalytic efficiency through charge separation. This charge transfer mechanism fundamentally differs from

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that of Type-II heterojunctions, where band alignment facilitates directional carrier migration for improved charge separation.

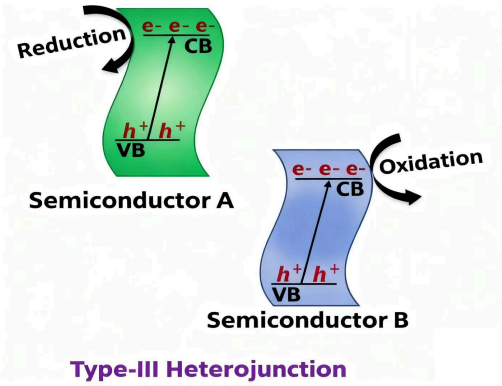


Figure 4. Mechanism of Type-III heterojunctions [8]

5. Prospects of photocatalytic technology in future applications

Photocatalytic technology demonstrates broad prospects in environmental governance. Coated on building exteriors and road surfaces, it can effectively decompose organic pollutants from vehicle emissions (e.g., formaldehyde, benzene derivatives) and inhibit PM2.5 formation. Significantly improving urban air quality. To advance large-scale implementation, further technological optimization and cost reduction are essential.

Future advancements will rely on deepened industry-academia-research collaboration and standardized systems. Photocatalytic technology is poised to become a low-cost, high-efficiency environmental solution, providing core support for urban sustainability and "Blue Sky Protection" initiatives.

Photocatalytic technology exhibits revolutionary potential in nutrient cycling and CO_2 resource utilization. By mimicking natural photosynthesis pathways, it achieves closed-loop carbon resource utilization. Photocatalysis decomposes organic matter from agricultural waste (e.g., straw, livestock manure) into small-molecule nutrients (e.g., ammonia, phosphates) while degrading pesticide residues. Reactive oxygen species (e.g., ·OH) cleave lignin-cellulose complexes, releasing mineral elements directly absorbable by crops and improving soil fertility. Novel photocatalysts leverage band engineering and interface design to enhance CO_2 reduction selectivity and efficiency.

Future innovations include photo-enzyme coupled systems that integrate CO_2 conversion with biofermentation for direct biofuel synthesis (e.g., bioethanol). Concurrently, artificial photosynthetic systems (e.g., Z-scheme heterojunction tandem reactors) enable solar to chemical to electrical energy cascade utilization, advancing "zero-carbon cycle" energy frameworks [11].

6. Conclusion

This analysis delineates the multifaceted landscape of contemporary photocatalysis, anchored by four pivotal material classes: metal oxides (e.g., WO_3 for visible-light activation), metal sulfides (e.g., ZnS), non-metallic semiconductors (e.g., defect-engineered g-C_3N_4), and metal-organic frameworks (MOFs with tailored active sites). Photocatalytic heterojunction technology optimizes charge behavior by coupling different semiconductor materials. In Type-I heterojunctions, band alignment causes carrier accumulation due to energy level wrapping, weakening redox capabilities. Type-II heterojunctions leverage staggered band structures to spatially separate electrons and holes,

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yet energy loss occurs during migration pathways. Type-III heterojunctions exhibit minimal charge transfer efficiency owing to non-overlapping bands, limiting practical applications. While this technology enhances pollutant degradation and energy conversion efficiency, it faces inherent constraints: failure in dark environments (e.g., sewer pipelines), low solar conversion efficiency (<5%), and material instability (e.g., photocorrosion). Future advancements require material optimization (e.g., defect engineering to tailor bandgaps) and system integration (e.g., hybrid photo-electro-biocatalytic systems) to enable scalable deployment in environmental and energy applications.

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