



EXPLORING CONCEPT AND MECHANISM OF PHOTOCATALYTIC DEGRADATION OF DYES

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ABSTRACT

Dye-contaminated wastewater treatment via photocatalytic degradation has recently emerged as a promising and eco-friendly option. Photocatalysts play a crucial role in this process by harnessing light energy to initiate chemical reactions. Photocatalysts hold significant potential for sustainable and effective dye degradation, contributing to the preservation of water resources and environmental sustainability. The indiscriminate release of dyes into the environment from various industries, particularly the textile sector, has led to severe ecological and health risks. To address this environmental challenge, photocatalytic degradation has emerged as a promising and sustainable solution.

Keywords: Degradation, Dyes, Semiconductor, Absorption, Electron

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3935

I. INTRODUCTION

Light energy and a photocatalyst are used to kick off chemical processes in a process known as photocatalysis. It has gained significant attention as a sustainable and environmentally friendly approach for various applications, including environmental remediation, energy conversion, and organic synthesis.

In photocatalysis, a photocatalyst, typically a semiconductor material absorbs photons from a light source, leading to the generation of electron-hole pairs. These excited charge carriers can initiate a range of chemical reactions, including redox reactions, degradation of pollutants, and synthesis of valuable compounds. The photocatalyst acts as a facilitator by providing a surface for reactant adsorption, promoting charge separation, and enhancing reaction kinetics.

Photocatalysis is a versatile and environmentally friendly process that utilizes light energy and a photocatalyst to drive various chemical reactions. It has garnered significant attention in fields such as environmental remediation, energy conversion, and organic synthesis. In photocatalysis, a photocatalyst, typically a semiconductor material, absorbs photons from

a light source and generates electron-hole pairs. These excited charge carriers initiate a series of redox reactions, leading to the transformation of target molecules. The photocatalyst acts as a catalyst by providing active sites for reactant adsorption, promoting charge separation, and accelerating reaction kinetics. Photocatalysis offers several advantages, including mild reaction conditions, high selectivity, and minimal generation of waste. Numerous industries have found uses for it, including pollution cleanup and hydrogen energy generation through water splitting, carbon dioxide reduction, and the synthesis of value-added chemicals. Ongoing research focuses on developing new photocatalytic materials, optimizing their properties, and exploring innovative reactor designs to advance the efficiency and applicability of photocatalysis. Overall, photocatalysis holds immense promise as a sustainable and efficient strategy for a wide range of chemical transformations and environmental remediation processes.

Photocatalysts play a crucial role in the degradation of dyes through photocatalysis, and several semiconductor materials have been investigated for this purpose. Among the



most commonly studied photocatalysts for dye degradation. TiO₂ and ZnO are widely used due to their excellent photocatalytic activity, stability, and low cost. These materials have a wide band gap, allowing them to absorb UV light and effectively degrade a range of dyes. WO₃ and ZnS are visible light-active photocatalysts, suitable for degradation under visible light irradiation. MOFs offer tunable structures and high surface areas, making them promising photocatalysts for dye degradation, while carbon-based materials exhibit unique properties such as high surface area and visible light absorption ability. The choice of photocatalyst depends on factors such as the dye to be degraded, available light wavelength, and system requirements. Ongoing research aims to further enhance the performance of these photocatalysts through surface modifications, doping, and co-catalyst incorporation, to achieve efficient and sustainable dye degradation.

II. FACTORS INFLUENCING PHOTOCATALYTIC DEGRADATION

Several factors influence the efficiency and effectiveness of photocatalytic degradation. Understanding and optimizing these factors is crucial for achieving efficient dye degradation. The key factors influencing photocatalytic degradation include:

Photocatalyst Properties

The properties of the photocatalyst play a vital role in determining its efficiency in dye degradation. Some important factors to consider include:

- **Band Gap Energy:** The photocatalyst's absorption spectrum is set by the energy of its band gap. In order to maximize the photocatalytic activity, it is best to optimize the band gap energy such that it corresponds with the dye's absorption spectrum.
- **Surface Area:** Increased contact between the catalyst and the dye solution, brought about by the larger surface area, leads to more efficient degradation.
- **Crystallinity:** The crystallinity of the photocatalyst affects its stability and the efficiency of charge carrier generation and separation. Higher

crystallinity generally leads to better photocatalytic performance.

- **Catalyst Loading:** The amount of photocatalyst in the system should be optimized to ensure sufficient catalytic activity without causing agglomeration or hindered mass transfer.

Dye Characteristics

The properties of the dye being degraded also influence the photocatalytic degradation process. Important dye characteristics to consider include:

- **Molecular Structure:** The molecular structure of the dye affects its adsorption onto the photocatalyst surface and the ease of degradation. Dyes with complex structures or aromatic moieties may require longer degradation times or additional treatments.
- **Concentration:** The concentration of the dye in the solution affects the reaction rate and the competition for active sites on the photocatalyst. Optimizing the dye concentration is crucial to achieve efficient degradation.
- **Dye Adsorption Affinity:** The affinity of the dye for the photocatalyst surface influences the adsorption and subsequent degradation process. Dyes with higher affinity for the photocatalyst surface tend to exhibit better degradation efficiency.

Solution Conditions

The conditions of the dye solution impact the photocatalytic degradation process. Key solution parameters to consider include:

- **pH:** The pH of the solution affects the surface charge of the photocatalyst and the ionization state of the dye. Optimizing the pH within a specific range can enhance the degradation efficiency.
- **Temperature:** The temperature influences the reaction kinetics and the rates of adsorption, desorption, and degradation. Controlling the temperature within an optimal range is



important for achieving efficient degradation.

- **Presence of Scavengers:** The presence of scavengers, such as dissolved oxygen or other reactive species, can compete with the dye for reactive radicals and reduce the degradation efficiency. Minimizing the presence of scavengers or optimizing their concentrations is crucial.

Light Source

The characteristics of the light source used for photocatalytic degradation affect the efficiency of the process. Important light source parameters include:

- **Wavelength and Intensity:** The wavelength of the light source should match the absorption range of the photocatalyst for efficient light absorption. Optimizing the light intensity ensures sufficient photon energy for promoting the photocatalytic reaction.
- **Spectral Distribution:** Utilizing light sources with a broad spectrum or combining multiple light sources can enhance the overall efficiency of the photocatalytic process by covering a wider range of wavelengths.

Understanding and optimizing these factors in the photocatalytic degradation process can lead to improved dye removal efficiency and the development of more sustainable and effective environmental remediation strategies.

III. CATALYSTS FOR PHOTOCATALYTIC DEGRADATION

Semiconductor Photocatalysts

The capacity of semiconductors to produce electron-hole pairs in response to light absorption makes them useful as photocatalysts. Some commonly studied semiconductor photocatalysts for photocatalytic degradation include:

- **Titanium Dioxide (TiO₂):** Because of its great efficiency, chemical stability, and cheap cost, TiO₂ is one of the most thoroughly investigated photocatalysts. The anatase phase has superior photocatalytic activity, however both phases may be used.

Dye is only one of several organic contaminants that may be effectively degraded by TiO₂.

- **Zinc Oxide (ZnO):** ZnO is another promising semiconductor photocatalyst with excellent photocatalytic properties. It possesses a suitable bandgap for absorbing UV light and has a high quantum efficiency. ZnO has shown remarkable performance in the degradation of various dyes and other organic pollutants.
- **Other Semiconductor Catalysts:** Besides TiO₂ and ZnO, several other semiconductor materials, such as iron oxide (Fe₂O₃), tungsten oxide (WO₃), and bismuth oxyhalides, have been investigated for photocatalytic degradation. These materials offer different bandgaps and unique photocatalytic properties, making them suitable for specific applications and targeted pollutant degradation.

Noble Metal-based Catalysts

Noble metal-based catalysts, particularly gold (Au) and silver (Ag) nanoparticles, have shown excellent photocatalytic activity due to their plasmonic properties. These catalysts exhibit surface plasmon resonance, which enhances light absorption and promotes efficient charge separation. Noble metal-based catalysts are effective in degrading dyes and other organic pollutants under visible light irradiation.

Co-catalysts and Modifications

In order to enhance the photocatalytic performance of semiconductor photocatalysts, co-catalysts and modifications are often employed. These include:

- **Metal Cocatalysts:** Co-catalysts such as platinum (Pt), palladium (Pd), and nickel (Ni) nanoparticles are deposited onto the surface of semiconductor photocatalysts to facilitate charge carrier separation and enhance catalytic activity. These metal cocatalysts act as electron or hole transfer mediators, leading to improved degradation efficiency.
- **Doping and Surface Modifications:**

3937



Doping of semiconductor photocatalysts with foreign elements or surface modifications with organic or inorganic species can alter their optical and electronic properties, enhancing their photocatalytic activity. Examples include nitrogen (N) or carbon (C) doping of TiO₂, which extends the light absorption range and reduces the recombination of charge carriers.

These catalysts, either alone or in combination, play a crucial role in the photocatalytic degradation of dyes by facilitating light absorption, charge separation, and reactive species generation. The choice of catalyst depends on factors such as targeted pollutant, light source, reaction conditions, and desired photocatalytic efficiency. Ongoing research aims to develop novel catalysts and explore synergistic effects between different catalysts to further improve the efficiency of photocatalytic degradation processes.

IV. PHOTOCATALYTIC DEGRADATION MECHANISMS

Photocatalytic degradation involves a series of interconnected mechanisms that enable the transformation of pollutants, such as dyes, under the influence of light and a photocatalyst. The key mechanisms involved in photocatalytic degradation are as follows:

Photon Absorption and Electron-Hole Pair Generation

When the photocatalyst is exposed to light energy, photons are absorbed by the catalyst's semiconductor material. Positively charged holes are left in the valence band as electrons are excited to the conduction band through this absorption. In doing so, electron-hole pairs are created, which serve as the primary reactive species for subsequent degradation reactions.

Charge Carrier Dynamics: Electron and Hole Migration

The photogenerated electrons and holes possess different reactivity and mobility. The photogenerated electrons in the conduction band are highly reducing species, while the holes in the valence band act as strong oxidizing agents. Both the electrons and holes migrate within the catalyst's lattice or along

the surface, seeking opportunities for reaction with adsorbed pollutants.

Adsorption of Pollutants onto the Photocatalyst Surface

The dye molecules present in the surrounding solution can adsorb onto the surface of the photocatalyst through various interactions such as electrostatic forces, hydrogen bonding, and π - π stacking. The adsorption step plays a crucial role in bringing the dye molecules in close proximity to the reactive sites on the photocatalyst surface, facilitating subsequent degradation reactions.

Reaction Pathways

Oxidation and Reduction Processes: Once the dye molecules are adsorbed onto the photocatalyst surface, the photogenerated electrons and holes initiate redox reactions. The photogenerated electrons (reducing agents) can directly react with the dye molecules, leading to the degradation of the dye by breaking down its molecular structure. The holes (oxidizing agents) can react with water or other species, generating highly reactive oxidative species, such as hydroxyl radicals (\bullet OH) or superoxide radicals (\bullet O₂⁻). These reactive species can attack the dye molecules, breaking them down into smaller, less harmful compounds.

Reactive Oxygen Species (ROS) Generation

The photogenerated holes can react with water molecules adsorbed on the catalyst surface, producing hydroxyl radicals (\bullet OH) through the process of water oxidation. Hydroxyl radicals are highly reactive species and play a crucial role in the degradation of dyes. They can directly react with the dye molecules or other organic intermediates, leading to the formation of simpler and less toxic byproducts.

Role of Intermediates and Byproducts in Degradation

During the photocatalytic degradation process, various intermediate compounds are formed as the dye molecules undergo sequential reactions. These intermediates may have different chemical properties compared to the parent dye, and their persistence and toxicity should be carefully evaluated. Further degradation of these intermediates by reactive species or additional photocatalytic cycles



leads to the formation of smaller and more readily biodegradable byproducts.

These mechanisms collectively contribute to the degradation of dyes through photocatalysis. The efficiency of the process depends on factors such as catalyst properties, light intensity, dye characteristics, and solution conditions. Photocatalytic systems for the removal of dye-contaminated wastewater and environmental contaminants may be made more effective by a better understanding of these processes and their optimization.

V. CONCLUSION

In conclusion, photocatalytic degradation of dyes holds great promise as a sustainable and efficient method for the treatment of dye-contaminated wastewater. Photocatalysts, such as titanium dioxide, zinc oxide, tungsten trioxide, zinc sulfide, metal-organic frameworks, and carbon-based materials, have demonstrated their effectiveness in degrading a wide range of dyes. These materials exhibit excellent photocatalytic activity, stability, and versatility, making them suitable for various applications. With continued advancements in photocatalysis, this technology has the potential to contribute significantly to the remediation of dye pollution, promoting cleaner and healthier environments.

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3939

