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Application of Semiconductor Nanomaterials in Water Pollution Treatment

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Abstract. Given the rapid advancement of industrialization and urbanization, multiple forms of water pollution have grown increasingly severe. Traditional water treatment technologies face challenges such as low treatment efficiency and secondary pollution. Semiconductor nanomaterial-based photocatalysis has emerged as a promising approach for green water pollution control. This paper adopts a literature review method to systematically explore the photocatalytic water purification mechanisms of semiconductor nanomaterials, summarize four material optimization strategies and review the research progress of classical photocatalytic materials such as TiO_2, ZnO, g-C_3N_4, and Nb-doped SnO_2. Studies indicate that Nb doping introduces oxygen vacancies and synergistically modifies the band structure, significantly improving the poor visible-light response and photocorrosion susceptibility of SnO_2, while enhancing the removal efficiency for organic pollutants, heavy metals, and pathogenic bacteria. At present, this technology is limited by material stability, actual water conditions, and engineering-scale production, making large-scale implementation difficult. In the future, theoretical simulations for material optimization, immobilized catalytic devices, and supporting reactors may facilitate the transition of photocatalytic water treatment technology from laboratory research to industrial applications.

Keywords: semiconductor nanomaterials, water pollution, photocatalyst, defect regulation

1. Introduction

With the acceleration of industrialization and urbanization, global water pollution has grown increasingly severe. The discharge of industrial wastewater, agricultural runoff, and domestic sewage has caused excessive levels of organic matter, heavy metals, pathogens, nutrients, and other pollutants in water bodies, threatening ecosystems and human health. Although traditional treatment technologies such as physical adsorption, chemical precipitation, and biological treatment have certain effects, they face bottlenecks including low efficiency, high cost, and secondary pollution. Therefore, it is urgent to develop efficient and sustainable new technologies for water pollution control [1].

Traditional water treatment mainly includes physical, chemical, and biological processes. Each type of method has obvious application limitations. Semiconductor nanomaterials, through photocatalytic action, can efficiently degrade organic pollutants in water into harmless small-molecule substances and also possess sterilization and disinfection functions, providing a new

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solution for water environmental remediation [2]. In recent years, researchers have continuously optimized the photocatalytic performance of semiconductor nanomaterials through various strategies, including band structure regulation, defect engineering, heterostructure design, and single-atom catalysis, thereby promoting their practical application in water treatment [3].

This paper focuses on modified tin dioxide-based semiconductor nanophotocatalytic materials. Nb doping constructs lattice oxygen vacancies, and through defect regulation and band engineering, the separation efficiency of photogenerated carriers is thereby optimized. The removal efficiency and microscopic reaction mechanisms of the material toward organic pollutants, heavy metal ions, and pathogenic microorganisms in water are systematically explored [2, 3]. Compared with traditional water treatment processes, Nb-doped SnO_2 can overcome shortcomings such as low visible-light utilization and severe photocorrosion [1]. This study improves the modification strategy of defect-type semiconductor catalysts, provides a new material option for the efficient treatment of refractory wastewater, and offers theoretical reference and experimental basis for the transition of photocatalytic technology from laboratory research to engineering applications [1].

2. Types of water pollutants and treatment mechanisms

Data from the United Nations Environment Programme (UNEP) show that approximately 80% of wastewater worldwide is discharged directly without effective treatment, leading to increased pollution of rivers, lakes, and coastal waters [4]. In wastewater treatment, semiconductor nanomaterials are widely recognized as green catalytic materials for water environment remediation due to their unique photocatalytic properties.

Under light irradiation, electrons in the valence band of a semiconductor are excited and transfer to the conduction band, generating electron-hole pairs. These further react with water and dissolved oxygen in the system to produce highly active reactive oxygen species such as $\cdot OH$ and $\cdot O_2^-$. Through strong oxidation-reduction effects, these active species destroy the chemical bonds of pollutants and eventually mineralize and decompose the pollutants, thereby achieving water purification [1]. According to the common categories of pollutants in water, photocatalytic removal targets can be divided into three types: organic pollutants, heavy metal ions, and pathogenic microorganisms.

Organic pollutants in water include dyes, antibiotics, phenols, agricultural organic pesticides, and other refractory components that are difficult to mineralize completely by traditional water treatment processes. Hydroxyl radicals generated by photocatalysis possess strong non-selective oxidizing ability and can gradually break the carbon-chain structures of organic pollutants, eventually converting them into harmless small molecules such as CO_2 and H_2O, thereby completely eliminating organic pollutant residues and potential toxicity [1, 2].

Heavy metals such as Cr(VI), Pb^{2+}, and Cd^{2+} in water cannot be oxidatively decomposed. Their detoxification mainly relies on the reduction effect of photogenerated conduction-band electrons. High-energy electrons directly reduce highly toxic high-valence heavy metals into low-toxicity or zero-valent solid substances, which are then separated from water through sedimentation, thus completing the removal of heavy metal pollutants [1, 3].

Pathogenic microorganisms such as Escherichia coli and other disease-causing bacteria in water can be inactivated by photocatalytically generated reactive oxygen species. Free radicals continuously damage bacterial cell membrane structures, oxidize intracellular proteins and genetic material, and block microbial metabolism and reproduction pathways, thereby achieving sterilization and disinfection of water [2].

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3. Structural design strategies of semiconductor nanomaterials

3.1. Band structure regulation

The band gap of a semiconductor determines its light absorption range and redox reaction capability. In the design of semiconductor photocatalysts, the band structure is a crucial consideration. However, due to the quantum confinement effect, the band gaps of nanostructures are usually widened, which fundamentally suppresses their photocatalytic performance [5]. To improve the photocatalytic performance of semiconductors, taking SnO_2 as an example, niobium doping combined with the introduction of oxygen vacancies into quantum dots enables synergistic dual-defect band engineering, thereby enhancing visible-light photocatalytic activity.

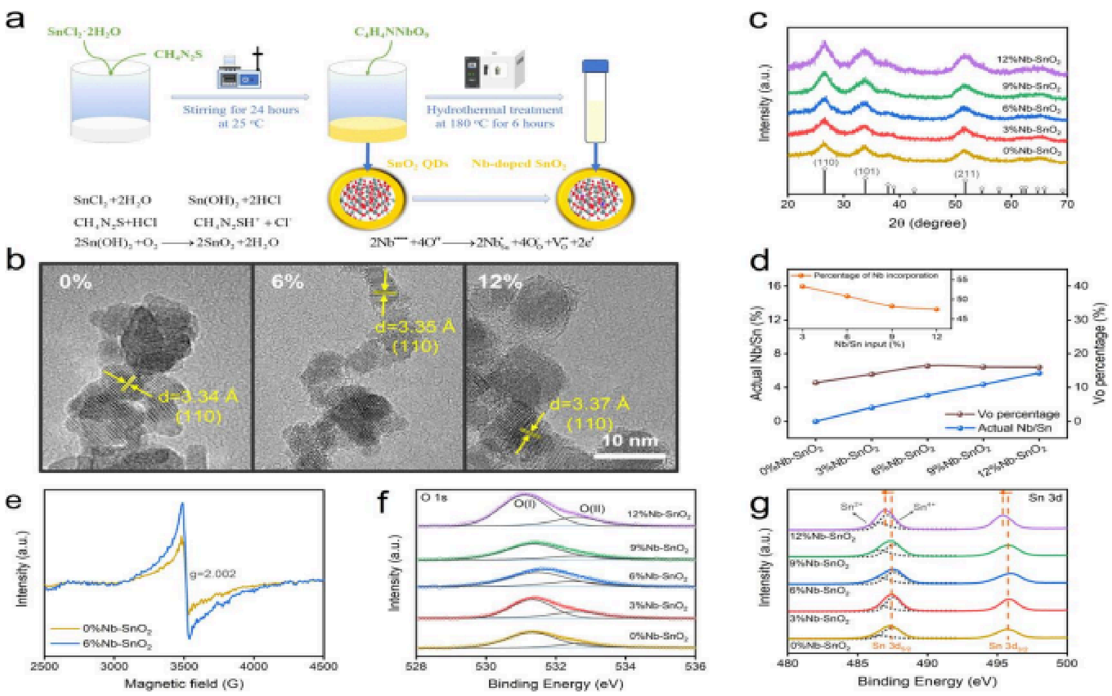

Figure 1. Synthesis and microstructural characteristics of Nb-induced V_o [5]

The prediction of material band structures using density functional theory (DFT) has been realized, and band gap engineering can be performed through DFT calculations [6]. Figure 1 shows the regulation of the band structure of the SnO_2 matrix by oxygen vacancy defects introduced through Nb doping. By comparing the DFTcalculated band structures of pure SnO_2 and samples with different Nb doping ratios, the changes in band gap width and shifts in band edges caused by doping modification are clearly shown. This reveals the internal mechanism of defect-induced band gap narrowing or widening and explains the essential reason for the optimization of photoelectric and catalytic properties from the electronic energy-level perspective.

After experimental measurements, DFT calculations can be employed to study the electronic properties of the band structure and energy levels of SnO_2 before and after Nb incorporation using density functional theory (DFT) [5].

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3.2. Defect engineering

In the field of environmental governance, water purification technologies are constantly evolving with the development of nanomaterial science. Among them, defect engineering, as a strategy for precisely regulating the physicochemical properties of materials, has shown great potential in improving the ability of semiconductor nanomaterials to treat water pollution. This is mainly attributed to its enhanced photocatalytic redox capacity and adsorption performance. The core of defect engineering lies in artificially introducing or eliminating vacancies, interstitial atoms, or impurity atoms in the crystal lattice to regulate the physicochemical properties of materials. In water pollution treatment, these defects are not merely "flaws," but functional "active sites." Taking MOFs as an example:

Although the metal centers of MOFs can provide potential active sites, their fully coordinated state causes metal ions to lack adsorption sites, thereby limiting their intrinsic catalytic activity. The absence of some organic ligands can lead to the formation of ligand-missing defects, altering the coordination environment around metal ions and exposing unsaturated metal sites, which further form Lewis acid centers or Brønsted acid centers. These acid centers play important roles in various heterogeneous catalytic reactions [7]. Controllable ligand defects can effectively optimize the electronic structure while maintaining crystallinity and porosity, enhancing the adsorption and activation capacity of reactants [7]. Density functional theory (DFT) calculations show that defect sites in $NiFc'_xFc_{1-x}$ promote the adsorption of oxygen-containing intermediates and improve catalytic activity. In addition, Xue et al. confirmed that linker defects can optimize the electronic structure of MOFs. Theoretical calculations indicate that this strategy significantly enhances OER performance by strengthening the adsorption of intermediates [7].

3.3. Heterostructure design

Heterostructure design can be combined with defect engineering and band engineering to achieve enhanced photocatalytic performance. Heterostructures are composite materials formed by stacking semiconductor materials such as graphene, hexagonal boron nitride, transition metal dichalcogenides, and black phosphorus. Among them, 2D/3D heterostructures have appealed many researchers due to the excellent electronic properties and broad spectral absorption capacity. However, structural defects are inevitably introduced during the synthesis of two-dimensional materials, which can significantly alter their intrinsic physical properties [8]. In the design process, the electronic and optical properties of heterostructures with different vacancy defects can be studied through first-principles calculations [8]. The heterostructures can be analyzed in detail from the perspectives of stability, electron density difference, band structure, density of states, absorption coefficient, and reflectivity [8]. These properties provide a theoretical basis for the design of semiconductor nanomaterials.

3.4. Construction of single-atom and surface active sites

By combining single-atom catalysis, construction of surface active sites, and design of porous structures with high specific surface areas, the photocatalytic performance of semiconductor nanomaterials such as $g\text{-}C_3N_4$ can be markedly enhanced [9]. Single-atom catalysis represents the limit of atomic utilization efficiency in heterogeneous catalysis. By anchoring isolated metal atoms onto semiconductor substrates, the electronic structure and surface reaction kinetics of materials can be substantially modified [10]. The specific surface area and pore structure directly determine the

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density of surface active sites and the contact efficiency with pollutants. Therefore, constructing porous g-C_3N_4 nanomaterials with high specific surface areas can enhance their performance in water treatment [9], as shown in Figure 2.

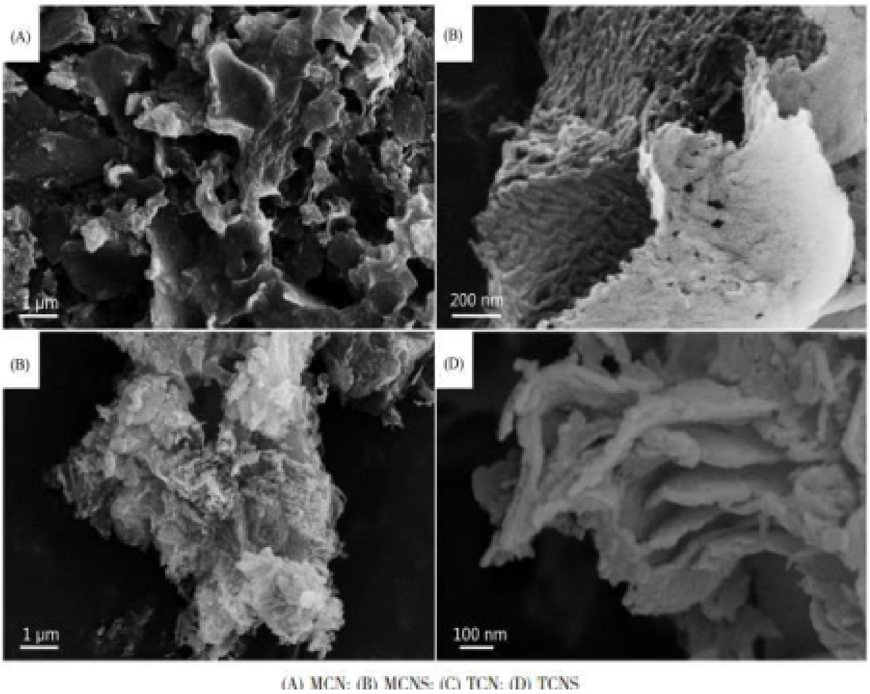

Figure 2. Schematic diagram of single-atom site construction and porous high-specific-surface-area g-C_3N_4 microstructure

4. Typical semiconductor nanomaterial systems

4.1. TiO_2-based materials and ZnO-based materials

Metal oxides have become promising photocatalysts owing to their adaptability to various structural architectures and morphologies, as well as their unique electronic structures. Among semiconductors, TiO_2 and ZnO are chemically stable, environmentally friendly, nontoxic, and lowcost. However, their low quantum efficiency and large band gaps limit their applications.

TiO_2 is an economical, non-corrosive, and widely studied photocatalyst. Heterojunctions can be used to improve the photodegradation performance of TiO_2. Mixing graphene oxide (GO) with TiO_2 can enhance the photocatalytic degradation performance of TiO_2.

Like TiO_2, ZnO is also an n-type semiconductor oxide and can serve as an alternative, although its potential has not yet been fully investigated. ZnO has a high exciton binding energy of 60 meV, a wide direct band gap of 3.37 eV, and deep ultraviolet absorption at room temperature. It exhibits excellent mechanical, electrical, optical, antibacterial, and photocatalytic properties, enabling its application in the efficient photocatalytic degradation of dyes. ZnO/Fe_2O_3 nanocomposites can degrade dyes more efficiently.

4.2. g-C_3N_4-based materials

g-C_3N_4 is a metal-free polymeric catalyst that has been widely investigated. Due to its high thermal and chemical stability, a suitable band gap of 2.7 eV, and visible-light response, it has been widely applied in hydrogen evolution, carbon dioxide reduction, removal of organic pollutants, and organic synthesis. The photocatalytic performance of g-C_3N_4 can be improved through heterojunction construction, crystal phase and facet control, doping, and other approaches.

Unlike other hard templates, CNTs can be easily removed and recovered by ultrasonic methods, allowing relatively simple preparation of porous g-C_3N_4 [9].

5. Conclusion

This study aims to systematically review the photocatalytic water purification mechanisms, material modification strategies, and mainstream catalytic systems of semiconductor nanomaterials, particularly focusing on the catalytic performance of niobium-doped tin dioxide modified by introducing oxygen vacancies. The analysis shows that the synergistic regulation of the band structure by niobium and oxygen vacancies can broaden the visible-light absorption range of the material and suppress photocorrosion, which supports the proposed view that dual-defect modification can simultaneously improve the removal efficiency of organic pollutants, heavy metals, and bacteria. This paper combines band regulation and defect engineering to analyze the catalytic mechanism of tin-based materials, thereby advancing the theory of semiconductor photocatalytic modification and filling the gap in comprehensive research on modified SnO_2 under composite polluted water conditions. It has direct practical reference value for preparing new photocatalytic materials and optimizing laboratory water treatment processes.

However, this paper relies solely on literature analysis and lacks independent experimental data. Future research can design gradient doping experiments to determine optimal preparation parameters, simulate real wastewater environments to investigate water quality interference mechanisms, and develop immobilized catalytic carriers to address the issue of powder catalyst recovery.

In summary, this study clarifies the internal logic by which synergistic defect modification improves photocatalytic performance and provides theoretical support for the industrialscale research and development of semiconductor catalytic materials for water pollution treatment.

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