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Design and Optimization of Doped Semiconductor-based Photocatalysts for Solar-Driven Water Decontamination

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Abstract: *The escalating crisis of water pollution, driven by industrial effluents, pharmaceuticals, and persistent organic pollutants, demands advanced remediation strategies. Semiconductor photocatalysis has emerged as a sustainable and efficient solution, harnessing solar energy to mineralize toxic contaminants. However, the practical application of pristine photocatalysts such as titanium dioxide (TiO_2) and zinc oxide (ZnO) is hindered by wide bandgaps, rapid electron-hole recombination, and limited visible-light absorption. This paper provides a comprehensive analysis of the design and optimization of doped semiconductor-based photocatalysts for solar-driven water decontamination. It systematically examines key material engineering strategies, including metal and non-metal doping, heterojunction construction, and defect engineering. The analysis demonstrates that these optimization techniques can extend light absorption into the visible spectrum, enhance charge separation, and increase reactive oxygen species (ROS) generation. Significant advancements in co-doped systems like N,S-CQDs and Ag_3PO_4 with Mo^{2+}-oxygen vacancy co-regulation have shown degradation efficiencies exceeding 90% for pollutants like tetracycline. Despite these breakthroughs, challenges remain in catalyst stability, scalability, and the economic feasibility of large-scale implementation. This review provides a critical assessment of these challenges and outlines future research directions, including the integration of machine learning for catalyst design and the development of sustainable synthesis pathways.*

Keywords: Photocatalysis, Doped Semiconductors, Water Decontamination, Band Gap Engineering, Heterojunctions, Solar Energy

I. INTRODUCTION

The rapid pace of industrialization and urbanization has led to alarming levels of water contamination, posing significant threats to ecosystems and public health worldwide . Persistent organic pollutants, including synthetic dyes, pharmaceuticals, pesticides, and phenolic compounds, are frequently discharged into water bodies from textile, agricultural, and chemical industries. These contaminants are often resistant to conventional treatment methods such as adsorption, coagulation, and biological degradation, leading to their accumulation in the environment . According to the World Health Organization, unsafe drinking water is responsible for hundreds of thousands of diarrheal deaths annually, highlighting the critical need for effective water treatment technologies .

In response to this global challenge, semiconductor-based photocatalysis has emerged as one of the most promising advanced oxidation processes (AOPs). This technology leverages light energy to generate reactive oxygen species (ROS) that can completely mineralize a wide range of organic pollutants into harmless substances like CO_2 and H_2O . Photocatalysis is considered a "green" technology due to its ability to utilize solar energy, its environmentally benign reaction conditions, and its potential for complete pollutant degradation without generating secondary waste .

Among the plethora of semiconductor materials, titanium dioxide (TiO_2) and zinc oxide (ZnO) have been extensively studied for their exceptional photocatalytic activity, chemical stability, non-toxicity, and low cost . However, the

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widespread implementation of these pristine photocatalysts is constrained by fundamental limitations. Their wide bandgaps (TiO_2 ~3.2 eV, ZnO ~3.3 eV) restrict their photoactivation to the ultraviolet (UV) region, which constitutes only a small fraction (3-5%) of the solar spectrum . Furthermore, the rapid recombination of photogenerated electron-hole pairs significantly reduces their quantum efficiency .

To overcome these challenges, extensive research has focused on the design and optimization of doped semiconductor-based photocatalysts . Doping, which involves the intentional introduction of foreign atoms (metals or non-metals) into the semiconductor lattice, is a proven strategy for tailoring its electronic and optical properties . This paper provides a detailed analysis of the key design strategies for doped photocatalysts, including metal and non-metal doping, the construction of heterojunctions, and defect engineering. It examines how these strategies contribute to enhanced visible-light responsiveness, improved charge separation, and ultimately, superior photocatalytic performance in solar-driven water decontamination.

II. DESIGN STRATEGIES FOR ENHANCED PHOTOCATALYTIC ACTIVITY

The design of high-performance photocatalysts is centered on overcoming the inherent limitations of pristine semiconductors. This is achieved through several sophisticated material engineering strategies that modify the band structure, surface properties, and charge carrier dynamics of the catalyst.

2.1 Doping with Metals and Non-metals

Doping is a cornerstone technique for modifying the electronic structure of semiconductor photocatalysts. By introducing impurities into the crystal lattice, the bandgap can be narrowed, creating intermediate energy levels that facilitate the absorption of visible light .

- **Metal Doping:** Transition metal ions (e.g., Fe, Cu, Mn, Mo, Sn) are frequently used as dopants for metal oxides like SnO_2, TiO_2, and ZnO . For instance, Mo^{2+} doping in Ag_3PO_4 introduces intermediate states that red-shift the optical absorption edge to the near-infrared region (700 nm) . Research on first and second series transition elements doped SnO_2 has shown that doping significantly enhances the degradation response in photocatalytic mechanisms by creating a high active surface area and tailoring the bandgap . A review by Liu et al. demonstrates that a novel Mo^{2+} and oxygen vacancy (OV) co-regulation strategy in Ag_3PO_4 enables highly efficient photocatalytic water remediation. The Mo^{2+} substitution for Ag^+ was found to be critical for band alignment and achieving 93% tetracycline degradation in just 30 minutes .
- **Non-metal Doping:** Doping with non-metals such as nitrogen (N), sulfur (S), boron (B), and phosphorus (P) has gained significant attention, particularly for carbon-based materials like carbon quantum dots (CQDs) . Non-metal doping effectively modulates the band structure of CQDs, enhancing electron mobility, improving charge separation, and boosting ROS generation. Nitrogen doping, for example, enhances electron-donating capabilities and charge separation, while sulfur doping tunes the bandgap and improves visible-light absorption . The synergistic effects of co-doping (e.g., N,S- or N,P-CQDs) have been shown to produce superior photocatalytic activity compared to single-element doping .

2.2 Heterojunction Construction and Nanocomposites

The construction of heterojunctions involves coupling two or more semiconductors with complementary band structures. This architecture is one of the most effective methods to spatially separate photogenerated electrons and holes, thereby suppressing recombination and preserving strong redox potentials .

- **Heterojunction Types:** Various types of heterojunctions, including Type-II, Z-scheme, and S-scheme, have been developed . A Z-scheme system mimics natural photosynthesis by facilitating electron transfer between two semiconductors, which maintains the strong reducing capability of one material and the strong oxidizing capability of the other . For example, a Z-scheme heterojunction can be formed between $Cs_3Bi_2I_9$ and Ag_3PO_4 to enhance charge separation and improve photocatalytic activity .

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- **Nanocomposites:** Nanocomposites combine nanomaterials to exploit synergistic effects. A study on the ZnO/BiOI composite demonstrated that pure ZnO shows no activity under visible light, but when coupled with BiOI, the composite achieved 78% degradation of methyl orange in 4 hours . Similarly, a $CdIn_2S_4/Bi_2MoO_6$ nanocomposite exhibited 93.7% degradation of levofloxacin, which was nearly twice the efficiency of its individual components, attributed to extended light absorption and reduced interfacial charge-transfer resistance .

2.3 Defect Engineering and Surface Modification

Defect engineering, particularly the introduction of oxygen vacancies (OVs), is another powerful approach to enhance photocatalytic performance. Oxygen vacancies can act as electron traps, extending carrier lifetime, and can also regulate the local charge distribution on the catalyst surface to promote the formation of reactive species . In the Mo-Ag_3PO_4 system, OVs were found to extend the carrier lifetime to 13.5 ns by acting as electron scavengers, fundamentally mitigating photocorrosion and enhancing stability .

Surface modification is crucial for improving the photocatalytic process. This includes surface tuning, facet exposure, and functionalization. These modifications can significantly enhance the adsorption of pollutants onto the catalyst surface and promote the selectivity of the degradation reaction .

III. OPTIMIZATION AND PERFORMANCE ANALYSIS

The optimization of photocatalytic systems is a multifaceted endeavor that involves not only material design but also the careful control of operational parameters and the integration of advanced technologies.

3.1 Key Operational Parameters

The efficiency of a photocatalytic reaction is highly sensitive to several operational parameters, and optimizing these can significantly boost performance .

- **Pollutant Type and Concentration:** The molecular structure of the pollutant dictates its susceptibility to attack by ROS . For example, the kinetics of degrading azo dyes differ significantly from those of pharmaceutical compounds.
- **Catalyst Loading:** The amount of photocatalyst in the system is critical. Optimal loading ensures sufficient active sites for reaction and light absorption without causing excessive light scattering that can reduce penetration.
- **Solution pH:** The pH of the solution influences the surface charge of the photocatalyst, the ionization state of the pollutants, and the formation of ROS. For instance, the generation of hydroxyl radicals can be more favorable in certain pH ranges.
- **Dissolved Ions and Water Matrix:** The presence of inorganic ions (e.g., carbonates, chlorides) and natural organic matter in real wastewater can act as scavengers for hydroxyl radicals, thereby reducing the overall efficiency . This "matrix effect" is a significant challenge for the practical application of photocatalysis in treating complex industrial effluents.

3.2 Advanced Characterization and Predictive Modeling

To rationally design and optimize photocatalysts, advanced characterization techniques are indispensable for understanding the relationship between a material's structure and its function . Techniques such as X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and electron microscopy (SEM, TEM) are standard for determining crystallinity, surface chemical states, and morphology.

Furthermore, integrating computational methods and predictive modeling is an emerging frontier in photocatalyst design. Density functional theory (DFT) simulations are increasingly used to predict the impact of doping on electronic structure and optical properties . The use of machine learning (ML) models is now being explored to predict optimal

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doping configurations and their impact on charge separation dynamics, accelerating the discovery of high-performance materials .

IV. CHALLENGES AND FUTURE DIRECTIONS

Despite the significant progress, several challenges continue to impede the widespread industrial adoption of photocatalytic water decontamination technologies.

4.1 Key Challenges

- **Scalability and Cost:** Many synthesis methods for doped and nanostructured catalysts are currently limited to lab-scale production and may be expensive or complex to scale up. Developing simple, scalable, and cost-effective synthesis routes is crucial .
- **Catalyst Stability:** Long-term stability and reusability remain a concern. Photocatalysts can suffer from photocorrosion, poisoning of active sites, and loss of co-catalysts, leading to a decline in activity over time .
- **Real-World Application:** The performance of photocatalysts in model laboratory experiments (often with distilled water and a single pollutant) does not always translate to real-world efficiency. Real wastewater contains a complex mixture of pollutants and scavengers that can significantly reduce photocatalytic activity .
- **Reactor Design:** Efficient photocatalysis requires reactor designs that maximize light distribution and mass transfer. Scaling up from small-batch reactors to pilot-scale systems introduces challenges related to light penetration depth and mixing .

4.2 Future Directions

The future of photocatalytic water treatment lies in the development of more robust, efficient, and sustainable systems, guided by interdisciplinary innovation.

- **Hybrid and Smart Systems:** Combining photocatalysis with other treatment processes, such as membrane filtration, adsorption, and ozonation, can create robust hybrid systems that address the limitations of individual technologies . The development of "smart" photocatalysts that can be activated and controlled on demand is also a promising avenue .
- **Sustainable Synthesis:** There is a strong push toward "green" synthesis methods. Utilizing agro-industrial waste or biomass (e.g., fruit peels or algae) as precursors for carbon-based photocatalysts aligns with circular economy principles .
- **Data-Driven Discovery:** Harnessing the power of artificial intelligence (AI) will be crucial. AI algorithms can be used to optimize synthesis parameters, predict catalytic performance, and accelerate the discovery of novel materials from a vast search space .

V. CONCLUSION

The design and optimization of doped semiconductor-based photocatalysts represent a significant leap forward in the development of solar-driven water decontamination technologies. Through strategies such as metal/non-metal doping, heterojunction construction, and defect engineering, researchers have successfully created materials that overcome the limitations of pristine semiconductors by extending light absorption into the visible spectrum and enhancing charge carrier separation. The impressive degradation efficiencies achieved against a wide array of recalcitrant pollutants demonstrate the immense potential of photocatalysis as a sustainable and effective advanced oxidation process.

REFERENCES

1. França, Y. K. de S., Pereira, K. S., Feitosa, Y. H. C., Marques, V. B., & Rodrigues de Souza, D. (2025). Titanium Dioxide (TiO2) and Photocatalysis: A Detailed Overview of the Synthesis, Applications, Challenges, Advances and Prospects for Sustainable Development. *Orbital: The Electronic Journal of Chemistry, 17*(4), 355-381. https://doi.org/10.17807/orbital.v17i4.23400

2. Shariq, M., AlGhamdi, G. S., Alotaibi, R., Almuqati, N. S., Toraba, M. A., & Albarqan, M. (2025). Design, synthesis, and structural engineering of carbon quantum dots and multifunctional N, P, B, S-doped CQDs for photocatalytic water purification. *Journal of Water Process Engineering*. https://www.sciencedirect.com/science/article/abs/pii/S2214714425015235
3. Anantharama, H., & Naveen Kumar, J. R. (2025). Review on Nanomaterial-Based Photocatalysis for Environmental Applications. *International Journal of Applied Engineering and Management Letters*.
4. Nongmaithem, M. S., Leishangthem, N., Das, J., & Singh, N. R. (2025). Multifunctional metal oxide photocatalysts for water purification: Advances in organic pollutant degradation and antibacterial applications. *Sustainable Materials and Technologies*. https://www.sciencedirect.com/science/article/abs/pii/S295035742500085X
5. Ramos, P., Sánchez, L., & Rodríguez, J. (2025). *Enhancing Photocatalytic Water Decontamination: Exploring the Efficacy of ZnO Nanorods in Advanced Treatment Processes*. Springer. https://link.springer.com/book/9783031825057
6. Liu, Y., Wang, B., Lv, D., Ma, H., Miao, Z. C., & He, Z. M. (2025). Mo-oxygen vacancy Co-regulation in Ag3PO4: Band alignment and adsorption optimization for high-efficiency photocatalytic water remediation. *Journal of Alloys and Compounds*. https://www.sciencedirect.com/science/article/abs/pii/S0925838825041143
7. Arora, S., & Dhiman, V. (2022). Recent Developments on I and II Series Transition Elements Doped SnO2 Nanoparticles and its Applications For Water Remediation Process: A Review. *Journal of Water and Environmental Nanotechnology*. http://www.jwent.net/article_253466.html
8. Taghavi, S. M., Rowley-Neale, S., Banks, C. E., Aminabhavi, T. M., & Ghaedi, M. (2026). Photocatalytic nanocomposites: mechanisms and influencing parameters to practical challenges. *Chemical Engineering Journal*. https://www.sciencedirect.com/science/article/abs/pii/S1385894726003839
9. (2024). Effective photocatalytic waste water treatment system using metal oxides semiconductors: A review. https://finna.fi/Record/theseus_centria.10024_506400
10. (2025). Surface-modified TiO_2 photocatalysts for emerging contaminants: Strategies for band gap tuning, cocatalyst synergy, and reactivity enhancement. *Journal of Photochemistry and Photobiology C: Photochemistry Reviews*. https://www.sciencedirect.com/science/article/abs/pii/S1387700325017071
11. Cole, S. (2025, December 2). Optimizing Photocatalytic Processes for Water Remediation: Strategies, Challenges, and Future Directions. *Environmental Chemistry and Science*. https://www.envchemsci.com/posts/optimizing-photocatalytic-processes-for-water-remediation-strategies-challenges-and-future-directions