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Review Paper

Nano-photocatalysis for Degradation of POPs, Dyes and Pharmaceuticals Using TiO_2, ZnO, and CuO Nano-catalysts- A Review

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ABSTRACT

The increasing contamination of water bodies by persistent organic pollutants (POPs), industrial dyes, and pharmaceutical residues has raised environmental and public health concerns due to their toxicity, persistence, and resistance to conventional water treatment technologies. Nano-photocatalysis using semiconductor nanomaterials such as titanium dioxide (TiO_2), zinc oxide (ZnO), and copper oxide (CuO) has emerged as a promising advanced oxidation strategy capable of degrading and mineralizing these recalcitrant organic pollutants under light irradiation. This review delivers a comprehensive analysis of nano-photocatalytic mechanisms, material design strategies (including doping, heterojunction engineering, and composite formation), and performance evaluations for degrading POPs, dyes, and pharmaceutical pollutants. Key challenges and future directions toward sustainable, visible-light-driven photocatalysis and practical implementation are also addressed.

1. Introduction

Water contamination by POPs (e.g., pesticides and industrial contaminants), synthetic dyes from textile effluents, and pharmaceutical residues (e.g., antibiotics and analgesics) is of global concern due to their environmental stability and ecological toxicity at trace levels (Paul & Ahmaruzzaman, 2025). Conventional treatment approaches such as biological processes, filtration, adsorption, and coagulation often fail to effectively remove these classes of pollutants, particularly at low concentrations and with complete mineralization (Paul & Ahmaruzzaman, 2025). In response, nanophotocatalysis has been extensively studied as a robust advanced oxidation process (AOP) that harnesses light-induced charge carriers in semiconductors to generate reactive oxygen species (ROS) capable of oxidizing organic contaminants to CO_2 and H_2O. Water pollution by organic contaminants such as persistent organic pollutants (POPs), dyes derived from textile and dyeing industries, and pharmaceuticals entering from healthcare and domestic sources remains a significant global environmental issue. These contaminants are frequently resistant to biodegradation, highly soluble, and pose toxicological risks even at trace concentrations. Traditional treatments (e.g., adsorption, coagulation, biological oxidation) often fall short in completely eliminating such pollutants without producing harmful by products. Photocatalysis using semiconductor nanomaterials has emerged as an effective advanced oxidation process to degrade these contaminants through light-induced generation of reactive oxygen species (ROS) such as hydroxyl radicals ($\bullet OH$) and superoxide anions ($O_2\bullet^-$). The semiconductor catalysts TiO_2, ZnO, and CuO have attracted considerable interest due to their tunable electronic structures, high surface areas, and ability to produce ROS under irradiation. However, inherent limitations such as wide band gaps limiting visible light absorption and fast electron-hole recombination have motivated extensive research on catalyst design and modification to improve efficiency and broaden applicability under solar or visible-light conditions.

The photocatalytic performance of a semiconductor depends critically on its band gap energy, light absorption range, and charge carrier dynamics. Anatase TiO_2, ZnO, and CuO are among the most widely studied photocatalysts due to their abundance, low toxicity, and strong oxidizing ability under photoactivation. However, limitations such as the wide band gap of TiO_2 and ZnO restricting them to UV activation and rapid electron–hole recombination have driven extensive

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research toward modification strategies to enhance visible light response, charge separation, and catalytic efficiency (Paul & Ahmaruzzaman, 2025; RSC Applied Interfaces Review, 2024)

2. Fundamental Mechanisms of Nano-photocatalysis

Photocatalysis begins with the absorption of photons with energy equal to or greater than the semiconductor's band gap, promoting electrons from the valence band (VB) to the conduction band (CB), creating electron–hole pairs (e^-/h^+). These charge carriers initiate redox reactions: photogenerated electrons reduce molecular oxygen to superoxide radicals ($O_2\bullet^-$), while holes oxidize water or hydroxide ions to hydroxyl radicals (•OH), both of which are potent oxidants for organic pollutant degradation (RSC Advances Comprehensive Review, 2025). Efficient photocatalysis requires (1) broad light absorption (ideally under visible light), (2) effective charge separation to prevent recombination, and (3) abundant active surface sites for pollutant adsorption and interaction with ROS. Strategies such as heterojunction engineering, doping with metal or non-metal ions, and integration with co-catalysts are critical to overcoming inherent material limitations, enhancing ROS generation, and improving degradation kinetics.

3. Titanium Dioxide (TiO_2) Photocatalysts

3.1 Properties, Benefits, and Limitations

Titanium dioxide (TiO_2) remains the most studied photocatalyst due to its chemical stability, low cost, biocompatibility, and strong oxidative potential. TiO_2 in the anatase crystalline phase typically exhibits superior photocatalytic activity compared with rutile due to its lower electron–hole recombination rate and favorable surface properties. However, its wide band gap (~3.2 eV) limits effective light absorption to the ultraviolet (UV) portion of the spectrum (<388 nm), which constitutes only ~5% of solar irradiance. This severely limits direct utilization of solar energy for environmental photocatalysis (RSC Applied Water Science Review, 2025). Moreover, rapid recombination of charge carriers significantly reduces quantum efficiency for pollutant degradation.

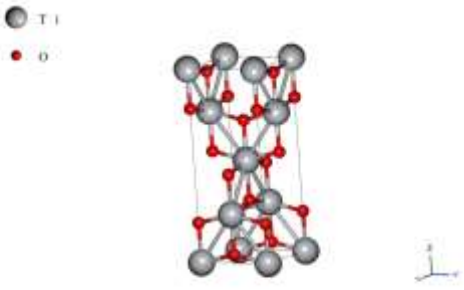

Fig.1 TiO_2 Crystal Structure

3.2 TiO_2 Modification Strategies

To improve visible-light responsiveness and suppress recombination, a variety of modification approaches have been developed.Doping with metal and non-metal elements: For example, Ag-doped TiO_2 hollow microspheres have shown enhanced removal rates of pharmaceutical compounds such as tetracycline hydrochloride under visible light, owing to improved charge separation and reduced band gap energy (RSC Applied Interfaces Review, 2024). Heterojunction formation: TiO_2 coupled with other semiconductors such as SnO_2 and SiO_2 has greatly improved degradation rates of antibiotics like ciprofloxacin and tetracycline by facilitating charge transfer across interfaces and expanding the light absorption window (Li et al., 2025). Composite and co-catalyst systems: Incorporation of carbonaceous materials such as reduced graphene oxide (rGO) or coupling with CdS has been shown to enhance ROS generation through improved electron mobility and extended photoresponse (Madduri & Kommalapati, 2024). These strategies systematically address TiO_2's intrinsic limitations and support high degradation efficiencies across diverse pollutant classes.

3.3 Photocatalytic Applications of TiO_2

TiO_2 and its modified forms effectively degrade industrial dyes (e.g., methyl orange, methylene blue), POPs, and pharmaceuticals in aqueous environments. For example, carbon-supported TiO_2 composites achieved near-complete degradation (>99%) of ceftriaxone and high chemical oxygen demand (COD) removal in pharmaceutical wastewater, attributed to enhanced charge separation and heterojunction effects (Applied Water Science Review, 2025). Moreover, TiO_2-based heterostructures have been incorporated with membrane systems to intensify contaminant removal while enabling catalyst recovery and reuse, demonstrating practical potential for wastewater treatment (Applied Water Science Review, 2025).

4. Zinc Oxide (ZnO) Photocatalysts

4.1 Photocatalytic Attributes of ZnO

Zinc oxide (ZnO) is a widely studied semiconductor with a wide band gap (~3.25 eV) and strong oxidative capability under UV light. ZnO nanoparticles typically exhibit high intrinsic photocatalytic activity due to efficient ROS generation and a high exciton binding energy, making them suitable for pollutant degradation. However, like TiO_2, ZnO suffers from rapid electron–hole recombination and limited visible-light absorption, which restrict practical solar-driven applications.

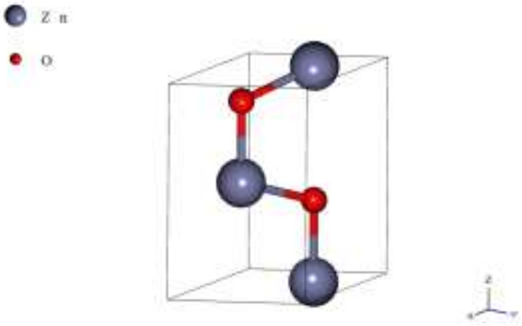

Fig. 2 ZnO Crystal Structure

4.2 Enhancement Strategies for ZnO

Recent research has focused on ZnO modifications to broaden light absorption and improve charge separation. Doping ZnO with elements such as Nb and co-dopants like Al/Cu has been shown to enhance photocatalytic performance significantly due to structural changes that create defect states and improve light harvesting (RSC Applied Interfaces Review, 2024; MDPI ZnO Co-doped Films, 2025). For instance, Nb-doped ZnO nanoparticles achieved ~93.2% degradation of tetracycline under visible light, demonstrating stability and recyclability (RSC Applied Interfaces Review, 2024). Other strategies include hydrothermal synthesis, which yields ZnO with high surface area and crystallinity, conducive to fast degradation kinetics for dyes and other pollutants (Springer Nature Link ZnO Review, 2025).

4.3 ZnO Applications in Pollutant Degradation

Biosynthesized ZnO nanoparticles have achieved complete elimination of methylene blue in as little as 60 min under light irradiation, demonstrating excellent activity and eco-friendly synthesis routes (PubMed ZnO Dyes, 2021). Modified ZnO systems have also shown promise in degrading pharmaceuticals and POPs, especially when engineered with complementary co-catalysts or dopants to improve ROS production and visible-light utilization.

5. Copper Oxide (CuO) Photocatalysts

5.1 Photocatalytic Potential and Challenges of CuO

Copper oxide (CuO) is a p-type semiconductor with a narrower band gap (1.2–1.9 eV), enabling absorption in the visible light region and potential for solar-driven photocatalysis. CuO's low band gap and cost-effectiveness make it an attractive material for environmental remediation. However, CuO often exhibits rapid electron–hole recombination and photo-instability that limit its standalone effectiveness (RSC Advances Comprehensive Review, 2025). Standalone CuO nanoparticles have achieved moderate dye degradation (e.g., methylene blue), but performance is greatly enhanced when integrated into heterojunction systems (ScienceDirect CuO@TiO_2)

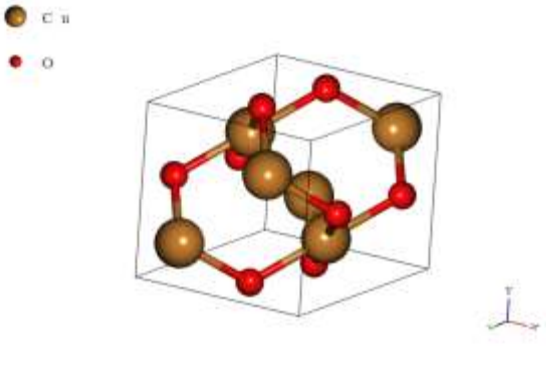

Fig.3 CuO Crystal Structure

5.2 CuO in Composite Photocatalysts

Forming heterojunctions with other semiconductors such as TiO_2 or ZnO helps alleviate charge recombination and expands photoresponse. For instance, CuO@TiO_2 composites exhibited ~83.9% degradation of methylene blue under xenon lamp irradiation, with repeated use showing stable activity, emphasizing heterojunction benefits for improved ROS production and pollutant degradation (ScienceDirect CuO@TiO_2, 2024). Similarly, green-synthesized CuO/ZnO nanocomposites demonstrated high methylene blue removal (>96%) with pH-dependent activity trends and ROS involvement in dye degradation, reinforcing the role of complex composite structures for enhanced photocatalysis (MDPI CuO/ZnO, 2025).

5.3 Electronic Band Structure

The catalytic behavior of Titanium dioxide (TiO_2), Zinc oxide (ZnO), and Copper(II) oxide (CuO) nano-catalysts is strongly dictated by their electronic band structures, which govern light absorption, charge excitation, and redox capability. TiO_2, particularly in anatase and rutile phases, possesses a wide band gap (~3.0–3.2 eV), with the valence band (VB) primarily composed of O 2p orbitals and the conduction band (CB) dominated by Ti 3d orbitals. The large band gap restricts absorption mainly to the ultraviolet region but positions the VB at sufficiently positive potentials to enable strong oxidative reactions, such as hydroxyl radical generation. Similarly, ZnO exhibits a comparable wide direct band gap (~3.2–3.4 eV), with Zn 4s states forming the CB and O 2p states forming the VB. Its direct band structure and high exciton binding energy (~60 meV) promote efficient electron mobility and fast charge transport, beneficial for photocatalytic and optoelectronic applications (Özgür et al.,). In contrast, CuO displays a much narrower band gap (~1.2–1.9 eV) arising from strong hybridization between Cu 3d and O 2p orbitals. This narrower gap enables visible-light absorption and intrinsic p-type conductivity due to copper vacancies, enhancing its applicability in solar-driven catalysis; however, the localized nature of Cu 3d states can increase electron–hole recombination if not properly engineered (Zhang et al., 103–107).

5.4CuO Electronic Band Structure

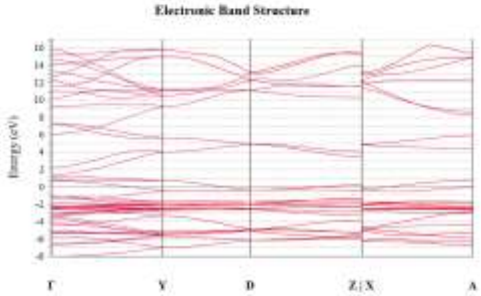

Fig.4 Electronic Band Structure of CuO

5.5 TiO₂ Electronic Band Structure

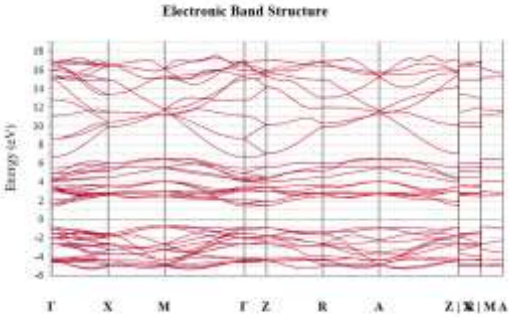

Fig.5 Electronic Band Structure of TiO₂

5.6 ZnO Electronic Band Structure

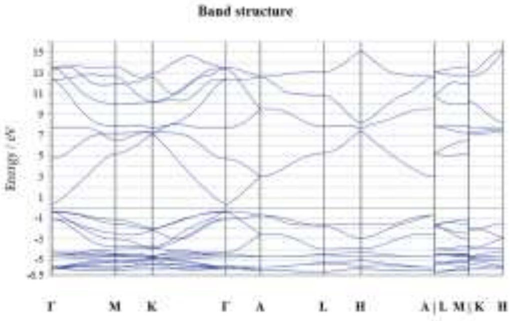

Fig.6 *Electronic Band Structure of ZnO*

5.7 Density of States (DOS)

The density of states (DOS) provides deeper insight into the distribution of electronic energy levels and their influence on catalytic performance. In TiO₂, the DOS near the valence band maximum is dominated by O 2p states, while the conduction band minimum consists largely of Ti 3d states, with relatively low intrinsic DOS at the Fermi level. This separation of states supports efficient charge separation but limits visible-light absorption without defect or dopant-induced mid-gap states (Fujishima, Rao, and Tryk). ZnO exhibits sharp DOS edges characteristic of a direct band gap semiconductor; the CB shows a strong contribution from delocalized Zn 4s states, which enhances electron transport, while the VB is primarily O 2p in character. The relatively low DOS near the band edges reduces carrier trapping but can also limit visible-range optical transitions unless modified by defects or doping (Özgür et al., 1255–1260). In CuO, the DOS is significantly influenced by narrow and localized Cu 3d bands that lie close to the Fermi level, producing a higher DOS in this region compared to TiO₂ and ZnO. This elevated DOS facilitates visible-light-induced transitions and interfacial charge transfer but may also introduce defect-related mid-gap states that act as recombination centers (Zhang et al., 103–107). Therefore, differences in orbital hybridization, band dispersion, and DOS profiles directly determine light absorption range, carrier lifetime, and overall catalytic efficiency in these metal-oxide nanomaterials.

5.8 CuO Density of States (DOS)

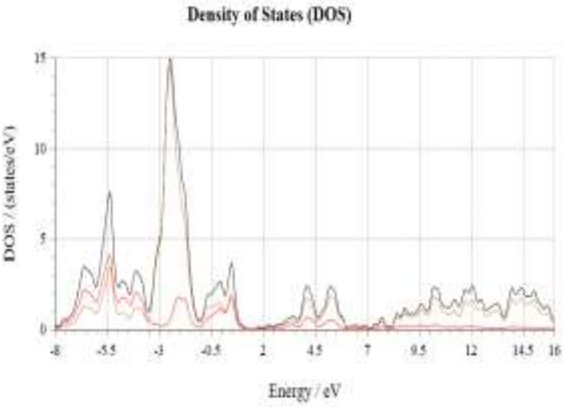

Fig.7 DOS of CuO

5.9 TiO_2 Density of States (DOS)

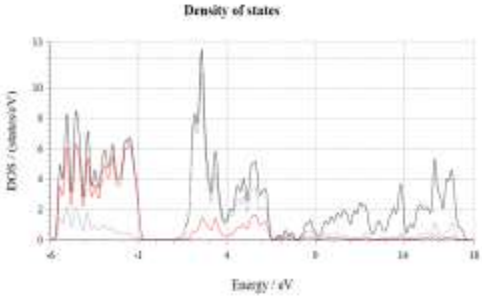

Fig.8 DOS of TiO_2

6. Comparative Performance: TiO_2, ZnO, and CuO Systems

Comparative studies indicate that while TiO_2 and ZnO are robust for UV-driven degradation, their catalytic activities under visible light require strategic modifications. CuO's narrower band gap facilitates visible-light absorption, but composite engineering is generally necessary to achieve competitive degradation efficiencies. Composite systems (e.g., TiO_2/ZnO, CuO/TiO_2, ZnO/CuO) often outperform individual oxides by combining broad spectral responses, enhanced charge separation, and improved surface reactivity (RSC Advances Comprehensive Review, 2025)

7. Photocatalytic Degradation of POPs, Dyes, and Pharmaceuticals

7.1 Dye Degradation

Various photocatalyst systems demonstrate efficient dye degradation: biosynthesized ZnO NPs achieved complete methylene blue removal within 60 min (PubMed ZnO Dyes, 2021), while TiO_2/rGO/CdS composites completely degraded methyl orange and methylene blue within hours, demonstrating optimized charge separation and synergy between components (Madduri & Kommalapati, 2024).

7.2 POPs Degradation

Advanced heterojunction composites have shown impressive removal of persistent pesticides and herbicides, with some novel nanostructures achieving nearly complete mineralization under visible light, reinforcing the potential for broader environmental applications (RSC Applied Interfaces Review, 2024).

7.3 Pharmaceutical Degradation

Photocatalytic systems based on modified TiO_2 and mixed metal oxides have demonstrated high degradation efficiencies for antibiotics such as ciprofloxacin, tetracycline, ibuprofen, and sulfamethoxazole, often exceeding 90% removal under optimized conditions (Springer Nature Link and Scientific Reports, 2025).

8. Challenges and Future Perspectives

Despite significant research progress, several practical challenges remain:

Visible-Light Activation: Many systems still require UV light; advancing visible-light activation is necessary for solar-driven applications.

Material Stability: Long-term stability and resistance to photocorrosion must be improved, particularly for copper-based systems. Scalability: Synthesis methods must be cost-effective and scalable for real wastewater treatment. Mechanistic Understanding: Detailed mechanistic insights into degradation pathways and by-product toxicity are critical for safe implementation.Future research should emphasize heterojunction engineering, plasmonic enhancement, and integration with hybrid treatment systems (e.g., membranes or adsorption) to achieve robust, sustainable photocatalytic water purification technologies.

9. Conclusion

Nanophotocatalytic degradation using TiO_2, ZnO, and CuO nanocatalysts presents a promising strategy to mitigate persistent organic contaminants, industrial dyes, and pharmaceuticals in water systems. Material modifications—such as doping, heterojunction formation, and composite design—significantly enhance photocatalytic performance by expanding light absorption and facilitating charge separation. Continued research into visible-light responsive photocatalysts and scalable synthesis methods will be key to translating laboratory advances into practical environmental applications.

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