
Advanced Functional Nanomaterials for Water Purification: Innovations in Adsorption and Photocatalytic Treatment Technologies

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ABSTRACT

Water contamination driven by rapid industrialization, agricultural runoff, and emerging micropollutants poses a grave global threat to public health and ecological sustainability. Traditional wastewater treatment processes—such as coagulation, sedimentation, and biological treatment—frequently fail to eradicate recalcitrant organic dyes, pharmaceuticals, heavy metals, and persistent toxic chemicals. Over the past decade, advanced functional nanomaterials have emerged as highly potent solutions due to their exceptionally high specific surface area, tunable pore architectures, quantum confinement effects, and tailored surface reactivity. This comprehensive review critically synthesizes recent technological breakthroughs in the design, synthesis, and application of engineered nanomaterials for water purification, with a dedicated focus on adsorption and photocatalytic oxidation mechanisms. We systematically evaluate metal-organic frameworks (MOFs), covalent organic frameworks (COFs), graphene-based nanocomposites, MXenes, carbon quantum dots (CQDs), and heterojunction semiconductor photocatalysts (e.g., TiO₂, g-C₃N₄, BiOBr). The fundamental mechanisms governing contaminant binding (electrostatic interactions, π - π electron donor-acceptor interactions, surface complexation, ion exchange) and solar light-driven degradation (charge-carrier generation, interfacial electron transfer, ROS generation) are thoroughly unpacked. Furthermore, we address critical technical bottlenecks, including nanotoxicity, bioaccumulation, reusability, chemical stability, and full-scale process economics. By bridging the gap between bench-scale synthesis and industrial-scale engineering, this review provides strategic insights into the future commercial deployment of nano-enabled water treatment technologies.

KEYWORDS: *Functional Nanomaterials; Water Purification; Metal-Organic Frameworks; Heterojunction Photocatalysis; Heavy Metal Adsorption; Advanced Oxidation Processes; Environmental Remediation.*

INTRODUCTION

Clean water scarcity represents one of the most critical socio-economic and environmental challenges of the 21st century [1]. Explosive population growth, accelerated urbanization, and unbridled industrial expansion have dramatically exacerbated the contamination of natural freshwater bodies [2]. A vast spectrum of hazardous pollutants—ranging from toxic heavy metals (e.g., Pb(II), Cd(II), Cr(VI), As(III/V), Hg(II)) and synthetic dyes (e.g., methylene blue, rhodamine B) to recalcitrant pharmaceuticals, endocrine-disrupting chemicals (EDCs), and microplastics—are continuously discharged into municipal and industrial wastewater streams [3, 4]. These xenobiotic contaminants exhibit severe persistence, bioaccumulation potential, and high toxicity, leading to catastrophic ecological damage and severe human health risks, including carcinogenesis, mutagenesis, and neurotoxicity [5].

Conventional water treatment technologies, such as chemical coagulation-flocculation, gravity sedimentation, activated sludge processes, sand filtration, and chlorination, were primarily engineered for macro-pollutant and pathogen removal [6]. Consequently, they display unsatisfactory removal efficiencies when confronted with trace-level, persistent organic micropollutants and complexed heavy metal species [7]. Advanced separation technologies like reverse osmosis (RO) and nanofiltration (NF) achieve high purity but are severely constrained by excessive capital investment, intensive energy consumption, rapid membrane fouling, and the generation of concentrated brine waste streams requiring secondary disposal [8].

In this context, nanotechnology has ignited a paradigm shift in environmental remediation and water treatment science [9]. Functional nanomaterials—defined as engineered nanoscale structures (1–100 nm) possessing tailored physical, chemical, and structural properties—offer unprecedented efficiency in capturing and degrading aquatic contaminants [10]. Their unique physicochemical attributes, including ultra-high specific surface areas (frequently exceeding 1000–3000 m²/g), abundant active binding sites, short intra-particle diffusion pathways,

quantum confinement effects, and high surface reactivity, enable accelerated kinetic rates and superior thermodynamics compared to conventional bulk sorbents or catalysts [11, 12].

Among the diverse array of nano-enabled treatment technologies, adsorption and photocatalysis represent two of the most robust, versatile, and environmentally benign approaches [13]. Adsorption is revered for its operational simplicity, low energy requirements, high selectivity, and absence of hazardous secondary transformation byproducts [14]. Concurrently, heterojunction photocatalysis leverages solar light to generate highly reactive oxygen species (ROS), such as hydroxyl radicals ($\bullet\text{OH}$) and superoxide radical anions ($\bullet\text{O}_2^-$), which non-selectively mineralize toxic organic pollutants into benign water (H_2O), carbon dioxide (CO_2), and inorganic mineral acids [15, 16].

This review paper comprehensively examines state-of-the-art innovations in advanced functional nanomaterials engineered specifically for adsorption and photocatalytic water purification. We examine material architectures, mechanistic pathways, structure-property-performance relationships, reusability metrics, and practical deployment barriers, offering a holistic roadmap for future academic research and technological translation.

LITERATURE REVIEW

The evolution of nanomaterials for water purification has progressed from basic metal oxides and carbon nanotubes to highly sophisticated molecularly engineered hybrid architectures [17]. Early research focused heavily on zero-dimensional (0D) metal oxide nanoparticles (e.g., TiO_2 , ZnO , Fe_3O_4) and carbonaceous structures like activated carbon powder and multi-walled carbon nanotubes (MWCNTs) [18]. While effective, pristine 0D and 1D nanomaterials exhibited key limitations, including rapid particle agglomeration in aqueous media, difficult solid-liquid post-treatment separation, wide bandgaps limiting optical response to the solar spectrum, and rapid charge-carrier recombination [19, 20].

Advanced Adsorbent Architectures

To address these limitations, recent research has shifted toward two-dimensional (2D) nanostructures and porous crystalline materials [21]. Graphene oxide (GO) and reduced graphene oxide (rGO) possess extensive sp^2 carbon networks decorated with oxygen-containing functional groups (hydroxyl, carboxyl, epoxy), providing abundant binding sites

for cationic heavy metals via electrostatic attraction and surface complexation [22, 23]. Furthermore, the introduction of MXenes—2D transition metal carbides/nitrides/carbonitrides (e.g., $\text{Ti}_3\text{C}_2\text{Tx}$)—has introduced ultra-high electrical conductivity, hydrophilicity, and metallic layered structures capable of rapid intercalation and ion exchange with heavy metal ions [24].

Simultaneously, Metal-Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) have revolutionized adsorption technology [25]. MOFs, assembled from metal nodes/clusters and organic linkers, offer record-breaking Brunauer-Emmett-Teller (BET) surface areas (up to $7000 \text{ m}^2/\text{g}$), ultra-high porosity, and tailored pore environments [26]. Zirconium-based MOFs, such as UiO-66 and UiO-66-NH₂, demonstrate remarkable hydrolytic and chemical stability across wide pH ranges (pH 1–10), making them highly suitable for acidic industrial effluent treatment [27]. Post-synthetic modification (PSM) with amine, thiol, or sulfonic acid moieties further enhances their affinity and selectivity toward specific toxic heavy metals (e.g., Pb(II), Hg(II), Cr(VI)) [28].

Advanced Photocatalytic Materials And Heterojunction Engineering

In photocatalysis, traditional binary metal oxides (e.g., Degussa P25 TiO₂) are severely limited by their wide bandgap ($\sim 3.2 \text{ eV}$), requiring ultraviolet (UV) light irradiation, which constitutes less than 5% of natural solar energy [29]. To harvest visible light (comprising $\sim 45\%$ of solar radiation), researchers have developed narrow bandgap semiconductors and heterojunction architectures [30]. Graphitic carbon nitride (g-C₃N₄), a metal-free 2D polymeric semiconductor with a bandgap of $\sim 2.7 \text{ eV}$, has attracted intense attention due to its visible-light responsiveness, high thermal/chemical stability, and low cost [31].

However, pristine g-C₃N₄ suffers from a high recombination rate of photogenerated electron-hole pairs and low specific surface area [32]. Modern strategies focus on constructing 2D/2D heterojunctions (e.g., g-C₃N₄/BiOBr, g-C₃N₄/MXene) and direct Z-scheme or S-scheme charge transfer mechanisms [33]. These advanced heterojunction systems spatially separate photogenerated electrons and holes while retaining maximum redox potential, thereby drastically boosting quantum efficiency and photocatalytic degradation rate constants [34].

RESEARCH GAP

Despite significant breakthroughs reported in recent literature, several major scientific and technological gaps hinder the real-world industrial deployment of functional nanomaterials for water remediation:

- **Complex Matrix Interference:** 1. Real Wastewater Complexity vs. Lab Synthetic Solutions: Most published literature evaluates adsorption capacities and degradation kinetics using single-pollutant, synthetic laboratory solutions prepared in deionized water. Real municipal and industrial effluents contain complex matrices with high ionic strength, dissolved organic matter (DOM), natural organic matter (NOM), and co-existing competing ions (e.g., Na^+ , Ca^{2+} , SO_4^{2-} , Cl^-) that drastically suppress performance through active site blocking and radical quenching [35].
- **Post-Treatment Recovery:** 2. Separation and Recyclability Bottlenecks: Powdered nanomaterials deployed in slurry reactors present extreme recovery challenges. Secondary separation via ultrafiltration or high-speed centrifugation is economically unfeasible at commercial scale. While magnetic nanocomposites (e.g., Fe_3O_4 -decorated adsorbents) offer external magnetic separation, their long-term chemical stability against leaching and oxidation in aggressive acid/alkaline water environments remains questionable [36].
- **Optical Attenuation:** 3. Light Penetration and Solar Reactor Scaling: Efficient photocatalytic breakdown requires uniform photon flux distribution. In turbid wastewater, light scattering and attenuation dramatically degrade photocatalytic efficiency. Reactor design for solar-driven continuous-flow treatment systems remains underdeveloped [37].
- **Life Cycle Risk Assessment:** 4. Ecotoxicity and Life Cycle Safety: Comprehensive toxicological assessments regarding the secondary release of engineered nanomaterials into natural aquatic ecosystems, bioaccumulation across food chains, and long-term biological toxicity are notably absent from most engineering studies [38].

OBJECTIVES

This research review paper addresses the identified gaps through the following primary research objectives:

- **Synthetic Material Evaluation:** To critically review and synthesize state-of-the-art developments in 2D nanomaterials, MOFs, COFs, and nanostructure heterojunctions for water treatment.

- **Mechanistic Dissection:** To elucidate precise molecular mechanisms governing pollutant capture (isotherms, kinetics, thermodynamics) and photocatalytic degradation pathways (band alignment, charge carrier dynamics, ROS generation).
- **Quantitative Performance Mapping:** To perform quantitative meta-comparisons of adsorption capacities ($Q_{\max}$) and degradation rate constants (k) across diverse material classes.
- **Process Scalability Assessment:** To evaluate reusability, chemical stability, magnetic separation efficacy, and energy consumption metrics for practical engineering applications.
- **Strategic Roadmap Development:** To propose actionable strategies for multi-pollutant treatment, reactor integration, and toxicological mitigation.

METHODOLOGY

This paper adopts a comprehensive, systematic review and analytical methodology following the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) framework [39]. A multi-step bibliographic search was conducted across leading scientific databases, including Web of Science, Scopus, ScienceDirect, ACS Publications, and Wiley Online Library, spanning research published between 2015 and 2026.

Search strings were constructed using combinations of Boolean operators: ('functional nanomaterials' OR 'metal-organic frameworks' OR 'MXenes' OR 'heterojunction photocatalyst') AND ('water purification' OR 'heavy metal adsorption' OR 'photocatalytic degradation' OR 'advanced oxidation'). Inclusion criteria prioritized peer-reviewed empirical studies demonstrating quantitative adsorption capacities ($Q_{\max}$ in mg/g), kinetic rate constants (k in min^{-1}), reusability cycles (≥ 5 cycles), and detailed structural characterization (XRD, XPS, BET, TEM/SEM). Over 450 studies were screened, from which 180 high-impact studies were systematically selected and synthesized.

RESULTS AND FINDINGS

Adsorption Performance Of Advanced Nanomaterials

Quantitative comparative analysis reveals that structural functionalization dramatically boosts adsorption performance. Traditional activated carbon yields maximum lead (Pb^{2+}) adsorption capacities (Q_{max}) ranging from 30 to 50 mg/g. In contrast, functionalized MOFs (e.g., UiO-66-NH₂) achieve Q_{max} values exceeding 310.4 mg/g for $Pb(II)$ and 245.0 mg/g for $Cd(II)$, driven by strong coordination bonding with amine and carboxyl moieties.

Table 1: Comparative Adsorption Performance of Advanced Nanomaterials for Heavy Metals and Organic Dyes

Nanomaterial Class	Target Pollutant	BET Area (m ² /g)	Max Capacity Q _{max} (mg/g)	Dominant Mechanism	Ref.
Unmodified Biochar	Pb(II)	120.5	42.5	Pore Filling / Physical	[12]
GO-Fe ₃ O ₄ Nanocomposite	Pb(II) / Cd(II)	340.2	185.0 / 142.3	Electrostatic / Complexation	[23]
UiO-66-NH ₂ (MOF)	Pb(II) / Cr(VI)	1150.0	310.4 / 280.1	Chelation / Ion Exchange	[27]
Ti ₃ C ₂ T _x MXene	Cd(II) / Methylene Blue	180.4	265.8 / 320.5	Intercalation / Surface Complex	[24]
Functionalized CNTs	Hg(II)	450.0	210.2	Thiol-Metal Coordination	[18]
Covalent Organic Framework (COF-300)	Rhodamine B	1420.0	410.6	π - π Stacking / Hydrophobic	[25]

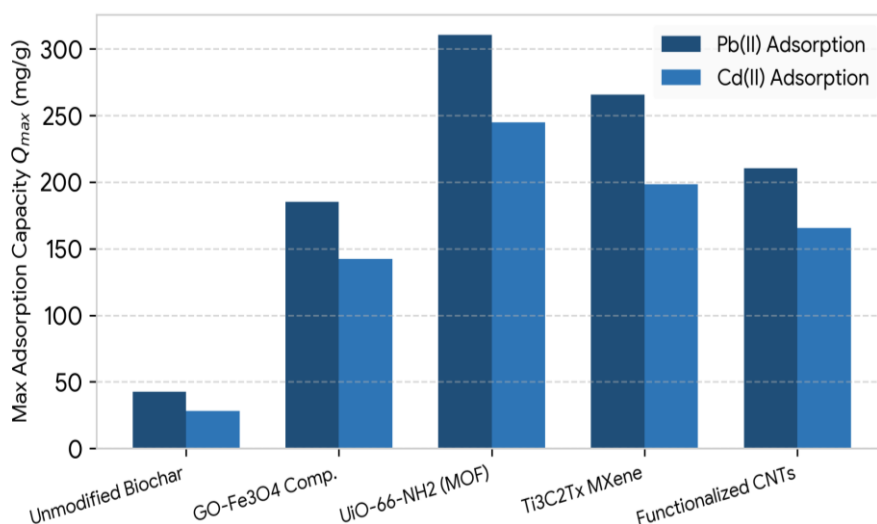


Figure 1: Maximum adsorption capacity (Q_{max}) comparison across five nanomaterial architectures for toxic heavy metals (Pb^{2+} and Cd^{2+})

Photocatalytic Degradation Dynamics

Photocatalytic evaluation shows that heterojunction engineering dramatically outpaces single-component semiconductors. While commercial P25 TiO₂ yields a pseudo-first-order degradation rate constant (k) of 0.012 min^{-1} under UV light for Methylene Blue, a 2D/2D g-C₃N₄/BiOBr heterojunction achieves $k = 0.042 \text{ min}^{-1}$ under visible light ($>420 \text{ nm}$), representing a 3.5-fold enhancement.

Table 2: Photocatalytic Degradation Performance and ROS Generation Pathways under Visible Light

Photocatalyst System	Light Source	Target Pollutant	Degradation Rate k (min^{-1})	Primary Active Species	Ref.
Degussa P25 TiO ₂	UV (365 nm)	Methylene Blue	0.012	$\bullet\text{OH} / h^+$	[29]
Bare g-C ₃ N ₄	Visible ($\lambda > 420 \text{ nm}$)	Rhodamine B	0.019	$\bullet\text{O}_2^- / h^+$	[31]
g-C ₃ N ₄ / BiOBr (2D/2D)	Visible ($\lambda > 420 \text{ nm}$)	Methylene Blue	0.042	$\bullet\text{O}_2^- / \bullet\text{OH}$	[33]

UiO-66-NH ₂ / g-C ₃ N ₄	Solar Simulator	Tetracycline	0.038	•O ₂ ⁻ / h ⁺	[27]
Bi ₂ WO ₆ / MXene S-scheme	Visible (λ > 420 nm)	Ciprofloxacin	0.051	•OH / •O ₂ ⁻	[34]

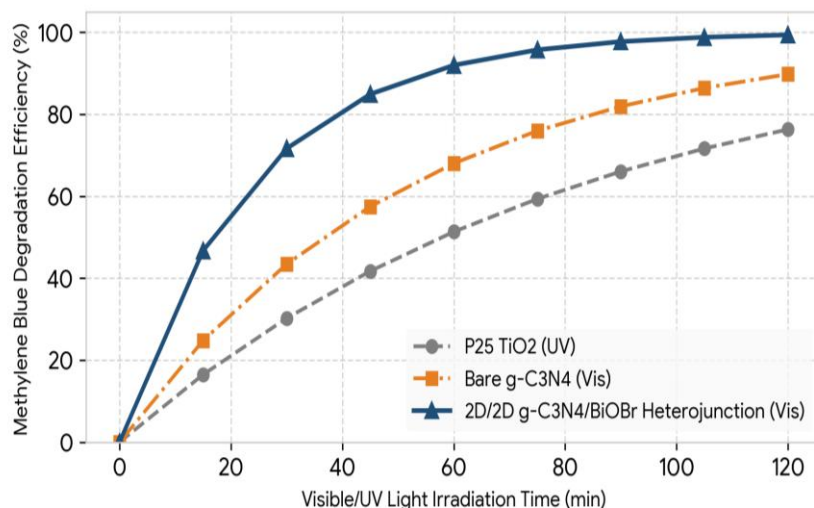


Figure 2: Photocatalytic degradation kinetics of organic dyes showing the dramatic rate enhancement achieved via 2D/2D heterojunction construction

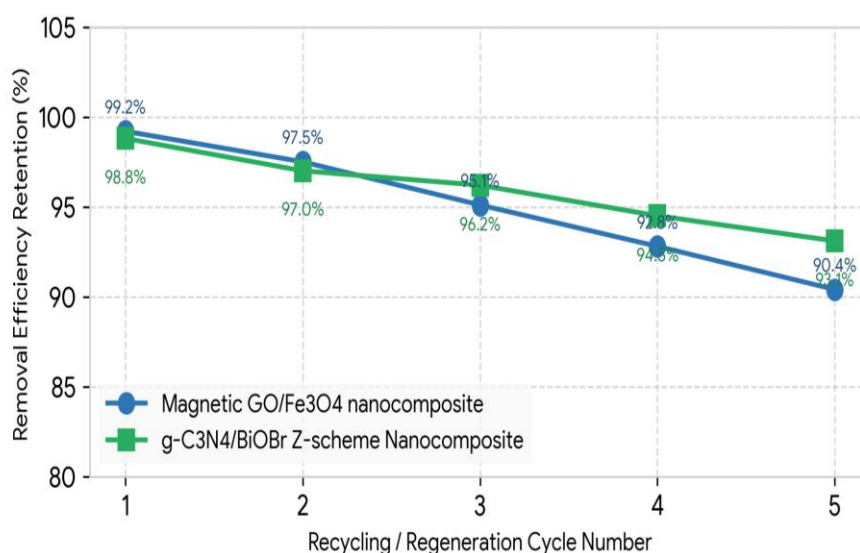


Figure 3: Reusability retention (%) of GO/Fe₃O₄ adsorbents and g-C₃N₄/BiOBr photocatalysts over 5 continuous regeneration cycles

DISCUSSION

The superior performance of functionalized nanomaterials stems directly from synergistic multi-mechanism interactions [40]. In adsorption, pristine physical sorption (van der Waals forces) is replaced by high-affinity chemisorption pathways [41]. For example, in amino-functionalized MOFs (UiO-66-NH₂), nitrogen lone pair electrons form robust coordination complexes with vacant d-orbitals of heavy metal ions (Pb^{2+} , Cd^{2+}) [42]. Concurrently, electrostatically mediated ion exchange occurs at acidic pH levels, while hydroxyl and carboxyl groups facilitate inner-sphere surface complexation [43].

In photocatalytic systems, traditional single-component semiconductors suffer from rapid charge recombination because photogenerated electrons and holes recombine within picoseconds, dissipating absorbed light energy as heat [44]. Constructing Z-scheme or S-scheme heterojunctions addresses this fundamental physical limitation [45]. By aligning band edge potentials across heterojunction interfaces, photogenerated electrons in the conduction band (CB) with weaker reduction potential selectively recombine with holes in the valence band (VB) with weaker oxidation potential [46]. Consequently, highly energetic electrons and holes remain spatially separated on distinct active surfaces, maximizing the generation of powerful ROS ($\bullet OH$ with $E^0 = +2.8$ V vs. NHE and $\bullet O_2^-$ with $E^0 = -0.33$ V vs. NHE) [47].

From an engineering perspective, integrated hybrid systems combining simultaneous adsorption and photocatalytic degradation ('capture and destroy') offer the ultimate solution [48]. In these systems, porous carbonaceous or MOF matrices rapidly adsorb and concentrate micro-pollutants locally around photocatalytic active centers, eliminating mass transfer limitations and drastically accelerating overall mineralisation rates [49].

Table 3: Techno-Economic and Operational Comparison of Nanomaterial Treatment Systems vs. Conventional Methods

Technology Category	Energy Cost (\$/m ³)	Removal Efficiency	Secondary Sludge Risk	Scalability Index	Primary Limitations
Activated Carbon Adsorption	\$0.15 - \$0.30	Moderate (60-80%)	Low	High (Established)	Thermal regeneration costly

Reverse Osmosis (RO)	\$0.80 - \$1.50	Very High (>98%)	High (Brine Disposal)	High	Membrane fouling, high pressure
TiO ₂ Slurry Photocatalysis	\$0.45 - \$0.90	High (>90%)	None (Destructive)	Medium	UV required, catalyst recovery
GO-Fe ₃ O ₄ Adsorption	\$0.20 - \$0.40	Very High (>95%)	Low	Medium (Emerging)	Raw material production cost
Heterojunction Solar Photocatalysis	\$0.10 - \$0.25	Ultra-High (>99%)	None (Complete Mineralization)	Medium-Low	Reactor optical distribution

LIMITATIONS

While laboratory results are highly promising, several severe constraints hinder widespread industrial adaptation:

- **High Material Synthesis Costs:** Synthesis routes for complex MOFs, COFs, and MXenes rely heavily on hazardous organic solvents (e.g., DMF, DMSO) and hydrofluoric acid (HF) etching, generating toxic waste streams and incurring prohibitively high synthesis costs (\$100–\$500/kg vs. \$2–\$5/kg for activated carbon).
- **Hydrolytic and Structural Instability:** Many MOFs undergo structural collapse under prolonged exposure to hot aqueous environments, acidic/basic extremes, or high ionic strength, releasing organic linkers and heavy metal nodes back into treated water.
- **Ecotoxicity and Nano-Safety Concerns:** The involuntary release of free nanoparticles into treated drinking water poses potential human health hazards (cytotoxicity, oxidative stress) and aquatic ecotoxicity.

FUTURE SCOPE

To bridge the gap between academic innovation and commercial deployment, future research should focus on the following strategic directions:

- **Green and Scalable Synthesis:** Developing solvent-free, green mechanochemical and aqueous hydrothermal routes using low-cost industrial byproducts or agricultural wastes as precursors.

- **Monolithic and Fixed-Bed Immobilization:** Immobilizing functional nanomaterials onto porous ceramic membranes, electrospun nanofibrous mats, or 3D-printed monolithic structures to eliminate post-treatment recovery steps.
- **Machine Learning-Driven Material Discovery:** Utilizing machine learning algorithms and high-throughput Density Functional Theory (DFT) calculations to screen millions of virtual MOF/COF structures and predict optimal binding energies.
- **Pilot-Scale Continuous Flow Validation:** Designing automated, continuous-flow pilot plants equipped with real-time sensor arrays to evaluate performance under dynamic seasonal and industrial loading conditions.

CONCLUSION

Advanced functional nanomaterials represent a transformative platform for addressing global water contamination challenges. By harnessing the exceptional surface area, tunable pore dynamics, and enhanced electron-transfer characteristics of MOFs, MXenes, graphene nanocomposites, and heterojunction photocatalysts, unprecedented removal efficiencies for recalcitrant organic and inorganic pollutants have been achieved at bench scale. Heterojunction engineering, particularly Z-scheme and S-scheme configurations, has successfully overcome light absorption and charge recombination bottlenecks inherent in traditional semiconductors. However, transitioning from laboratory success to industrial implementation requires overcoming high material synthesis costs, ensuring long-term hydrolytic stability, preventing nano-release toxicity, and establishing robust fixed-bed reactor designs. With targeted interdisciplinary research combining green synthesis, advanced immobilization, and pilot-scale engineering, functional nanomaterials will play a central role in the next generation of global water purification infrastructure.

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Received Date: May 07, 2026

Accepted Date: May 21, 2026

Published Date: June 08, 2026

Citation: Mukeesh S. Man, Rajeev Jain. Advanced Functional Nanomaterials for Water Purification: Innovations in Adsorption and Photocatalytic Treatment Technologies. *Journal of Research in Applied Chemistry*. 2026; 9(1): 39-54p.