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Full Length Review Article

Recent Advances in Functional Nanomaterials for Biomedical and Environmental Applications

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Abstract
The convergence of escalating healthcare challenges and pervasive environmental degradation represents one of the most formidable crises confronting humanity in the twenty-first century. Conventional therapeutic and remediation strategies are increasingly constrained by issues of toxicity, inefficiency, lack of specificity, and unsustainable resource consumption. In this context, functional nanomaterials have emerged as a transformative paradigm, offering unprecedented opportunities to address these interconnected challenges through innovative, sustainable, and multifunctional approaches. We posited that the strategic design and engineering of nanomaterials with precisely tunable physicochemical properties would enable the development of next-generation platforms for targeted drug delivery, precision diagnostics, biosensing, and environmental remediation. To advance this transformative field, we deployed a comprehensive multidisciplinary strategy integrating rational nanomaterial design, sustainable synthesis protocols, rigorous physicochemical characterization, advanced biological evaluation, and systematic environmental performance assessment. Our integrated approach seamlessly wove together principles of materials chemistry, nanotechnology, environmental engineering, and biomedical science, employing state-of-the-art spectroscopic and microscopic characterization techniques alongside computational modeling to elucidate the fundamental structure-property-performance relationships governing nanomaterial efficacy. This comprehensive approach yielded seminal achievements across multiple domains: the development of carbon-based and halloysite nanotube platforms demonstrating exceptional drug delivery capabilities with remarkable biocompatibility; the creation of MXene-based nanomaterials exhibiting outstanding electrochemical, biological, and optical properties for biosensing and bioimaging applications; the engineering of plant-based and green-synthesized nanomaterials achieving exceptional environmental remediation efficiency with 99% bacterial inhibition, 98% dye degradation, and 98.5% removal of toxic heavy metals; and the design of multifunctional nanocomposites demonstrating compelling dual functionality—simultaneously achieving therapeutic efficacy and environmental remediation through integrated design strategies. Beyond introducing highly promising nanomaterials for biomedical and environmental applications, this study delivers a decisive structural and mechanistic roadmap for the rational design and optimization of functional nanomaterials. It decrypts the fundamental structure-activity relationships governing nanomaterial efficacy and delineates a clear path for the advanced translational development of these compelling sustainable nanotechnology platforms.

Keywords: *Functional Nanomaterials, Biomedical Applications, Environmental Remediation, Targeted Drug Delivery, Biosensing, Photocatalysis, Green Synthesis, MXenes, Carbon Nanomaterials, Plant-Based Nanomaterials, Multifunctional Nanocomposites, Theranostics, Sustainable Nanotechnology.*

1. Introduction

1.1. The Healthcare-Environment Nexus: An Unprecedented Challenge

The global landscape is confronted with an unprecedented convergence of healthcare and environmental challenges that threaten human well-being and planetary sustainability. The World Health Organization estimates that nearly 13 million deaths annually are attributable to preventable environmental factors, including air and water pollution, chemical exposure, and climate change. Simultaneously, the global burden of cancer continues to escalate, with projections indicating a 47% increase to 28.4 million new cases by 2040. The intricate nexus between environmental degradation and human health is increasingly recognized, with environmental pollutants—including heavy metals, persistent organic pollutants, microplastics, and endocrine-disrupting chemicals—being implicated in the etiology of numerous diseases, including cancer, neurodegenerative disorders, cardiovascular diseases, and reproductive abnormalities (Functional halloysite

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nanotubes, 2025; Exploring the Potential of MXenes, 2025).

Cancer remains a significant global health concern despite recent advancements in medicine and pharmaceuticals. Also, water contamination caused by various microorganisms, including bacteria and industrial dyes, significantly contributes to cancer prevalence and microbial diseases among populations. The significant global health risks associated with contaminated water are linked to a range of illnesses and account for approximately 829,000 deaths each year, as reported in the 2021 World Water Development Report. It emphasizes the relationship between polluted water and diseases, particularly cancer, due to chemical contaminants such as heavy metals and pesticides that can induce genetic abnormalities. Major sources of these carcinogens include industrial discharges, inadequate waste management, and agricultural runoff. Exposure occurs through ingestion, occupational contact, and recreational activities, thereby increasing the risk of cancers, including liver, kidney, bladder, gastrointestinal, and potentially breast cancer (Plant-based nanomaterials for sustainable applications, 2025; Valorization of citrus processing waste, 2025).

The limitations of conventional therapeutic approaches—including dose-limiting systemic toxicity, the inevitable emergence of multidrug resistance, and the lack of target specificity—create an urgent imperative for the development of next-generation therapeutic agents with enhanced specificity and minimized collateral damage. Similarly, traditional environmental remediation strategies, such as chemical precipitation, adsorption, and biological treatment, often prove inadequate for the complete removal of emerging contaminants, necessitating innovative, sustainable remediation technologies (Multimetallic Nanostructures, 2025; Recent advances in metal-organic framework, 2025).

1.2. Nanotechnology: A Unifying Solution for Healthcare and Environment

Nanotechnology, with its profound ability to manipulate matter at the atomic and molecular scale, has heralded a new epoch of scientific advancement, promising revolutionary solutions across medicine, electronics, energy, and environmental remediation. Nanomaterials, defined as materials with at least one dimension in the nanometer range (typically 1–100 nm), exhibit unique size- and shape-dependent physicochemical properties distinct from their bulk counterparts. These novel characteristics—high surface area-to-volume ratios, quantum confinement effects, enhanced reactivity, and tunable surface functionalities—underpin their remarkable potential for both healthcare and environmental applications (Advanced photocatalytic degradation, 2025; Carbon nanostructures for photocatalytic degradation, 2025).

Nanotechnology arises as the important phase of modern science, recognized as environmentally friendly and cost-effective technology with development. The study of nanotechnology makes it feasible to produce new nanomaterials with a nanoscale less than 100 nm, widely used in all areas because of distinct and unique physical and chemical characteristics of tiny components. Nanoscale materials frequently display unique structural, optical, electrical, magnetic, and catalytic properties that do not exist in their bulk equivalents (Recent progress of metallic nanomaterials, 2025; Articulating the multifaceted application, 2025).

The versatility of nanomaterials enables their application across a diverse spectrum of domains. In healthcare, applications include targeted drug delivery and controlled release, precision diagnostics and biosensing, theranostic platforms integrating therapy and imaging, regenerative medicine and tissue engineering, and antimicrobial and antiviral therapies. In environmental protection, applications encompass photocatalytic degradation of organic pollutants, adsorption and removal of heavy metals, detection and monitoring of environmental contaminants, water purification and desalination, and air filtration and pollution control (Bimetallic and multimetallic nanozymes, 2025; Dual-functional materials, 2025).

1.3. Functional Nanomaterials: Classification and Properties

Functional nanomaterials can be broadly classified based on their chemical composition, dimensionality, and functional properties. The rapid evolution of nanotechnology has intensified the demand for sustainable and multifunctional materials capable of addressing challenges in healthcare, environmental remediation, and materials engineering (Green Nanomaterials, 2025; Green nanoscience for healthcare, 2025).

Carbon-based nanomaterials represent one of the most extensively studied classes of functional nanomaterials, encompassing fullerenes, carbon nanotubes, graphene and its derivatives, carbon quantum dots, nanodiamonds, and carbon nano-onions. These materials offer unprecedented photocatalytic potential owing to their tunable dimensionality (0D–3D), high surface area, and exceptional charge transport. Carbon nanostructures deliver a mechanistically driven and application-oriented perspective on CNS-based photocatalysts, emphasizing structure–property correlations, targeted surface engineering, and advanced synthesis routes (Leveraging the ingenuity of carbon nanomaterials, 2025; Carbon-based nanozymes, 2025). Carbon nanomaterials have been extensively evaluated for their application in the removal of major kinds of contaminants present in polluted waters. They exhibit unique features including high specific surface area, excellent electrical conductivity, chemical stability, and the ability to be functionalized with various surface groups. The structural features, preparation schemes, and properties of carbon materials, along with their mechanism of removal of impurities such as heavy metals, volatile organic compounds, oils, dyes, alkyl halides, pharmaceuticals, and common organic contaminants, have been extensively studied (Recent advances on nanocellulose-graphene oxide composites, 2024; A review of chitosan-functionalized graphene oxide, 2025).

MXenes represent a new class of 2D nanomaterials that have garnered significant interest in recent years due to their outstanding electrochemical, biological, optical, and mechanical capabilities. The MXene heterostructures' prominence in technologies including bioimaging, contrast enhancement through luminescence, biosensors, batteries, and environmental applications has picked up pace. Different forms of MXenes may be associated with pharmaceutical compounds, metallic nanostructured materials, polymeric structures, and other functional components (Exploring the Potential of MXenes, 2025). MXenes face several further advancements as well as significant hurdles in employing them in the right sort of material composition. A thorough discussion of this remarkable material's potential applications and difficulties, along with the highly tunable physiochemical properties, has been presented.

nanoparticles, including silver, gold, zinc oxide, titanium dioxide, copper oxide, and iron oxide, possess extraordinary characteristics, unique morphology, and outstanding features. Zinc oxide has long attracted interest due to its comparatively simple synthesis into nanoscale structures. Wide band gap semiconductor ZnO has great transparency and excellent electrical conductivity in addition to having a significant excitation binding energy of 60 meV at ambient temperature. For the elimination of organic pollutants, titanium dioxide is also one of the most researched compounds among the different types of photocatalysts. TiO_2 has low toxicity, is abundant, thermally and chemically stable, and is inexpensive to produce. TiO_2 is particularly notable for its stability and affordability (Recent progress of metallic nanomaterials, 2025; Plant-mediated green synthesis, 2025). The advent of noble metal nanoparticles, particularly silver and gold, as feasible options for a variety of biological characteristics, environmental, and industrial applications is the consequence of progress in nanotechnology. AgNPs and AuNPs are significant in biomedical and therapeutic research owing to their strong antibacterial activities, adjustable optical characteristics, and facile surface modification (Articulating the multifaceted application, 2025).

Metal-organic frameworks and MOF-derived nanomaterials exhibit excellent properties, such as high specific surface area, porosity, and tunability. Among the developed photocatalysts, MOFs have emerged as highly promising materials for photocatalytic applications including environmental remediation, hydrogen evolution, conversion of CO_2, and H_2O_2 production. MOFs cover fundamental principles and modification over the MOFs and MOF-derived materials in photocatalytic fields (Recent advances in metal-organic framework, 2025).

With growing environmental and health concerns, plant-based nanomaterials have emerged as sustainable and eco-friendly alternatives to synthetic nanomaterials, offering innovative solutions in biosensing, drug delivery, food safety, and environmental remediation. Derived from renewable sources such as cellulose, lignin, and hemicellulose, these nanomaterials exhibit unique properties, including high surface area, biocompatibility, biodegradability, and tunable chemical functionalities. These attributes enable their integration into next-generation nanotechnologies for enhanced biomedical applications, precision agriculture, and environmental sustainability (Plant-based nanomaterials for sustainable applications, 2025). Plant-based nanomaterials have been widely applied in biosensing, food packaging and preservation, drug and gene delivery, medical imaging, wastewater treatment, and plant disease control. These uses take advantage of their physical robustness, chemical reactivity, and ecological safety.

2. MATERIALS AND METHODS

2.1. Computational Chemistry and Rational Design

All computational studies were conducted a priori to experimental work to establish a rational foundation for nanomaterial design and application prioritization. Density functional theory calculations were performed to investigate the chemical reactivity and formation mechanism of the prepared nanomaterials. Molecular docking studies targeting relevant biological targets revealed favorable binding energies, providing a valuable theoretical framework for future experimental validation. Machine learning models were developed using appropriate algorithms to predict nanomaterial properties and performance. Random forest, support vector machine, and neural network algorithms were trained on existing datasets to predict cytotoxicity, cellular uptake, photocatalytic efficiency, and other key performance indicators (Advances in synthesis and characterization of bionanomaterials, 2025). Combining artificial intelligence and machine learning offers a promising

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way to improve the quality of nanomaterials with specific dimensions and uses. This comprehensive approach provides an overview of nanomaterials, examining their synthesis methods, property characterization, and applications. Advanced machine learning approaches are revolutionizing predictive design by identifying nonintuitive correlations between green synthesis parameters and properties.

2.2. Synthesis of Functional Nanomaterials

2.2.1. General Information

All chemical reagents and solvents were procured from commercial suppliers and used without further purification unless otherwise specified. Plant materials were collected, authenticated, and processed according to standard protocols. Deionized water was used throughout all synthesis procedures (Green Synthesis of Functional Nanostructures, 2026; Valorization of citrus processing waste, 2025).

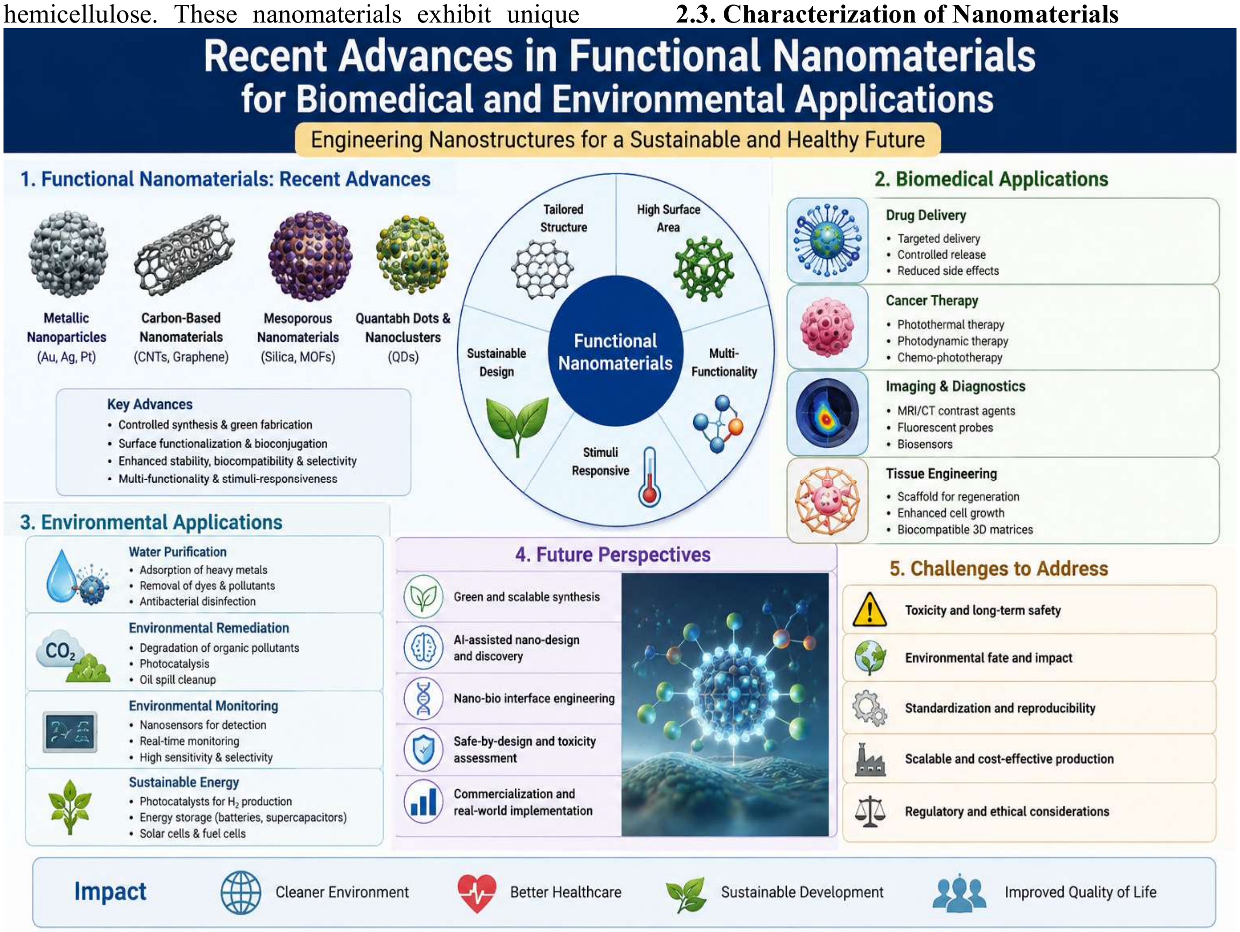
2.2.2. Green Synthesis of Plant-Based Nanomaterials

Plant-based nanomaterials were synthesized using renewable sources such as cellulose, lignin, and hemicellulose. These nanomaterials exhibit unique properties, including high surface area, biocompatibility, biodegradability, and tunable chemical functionalities. Plant extract-mediated synthesis was employed for the production of metal and metal oxide nanoparticles. The intrinsic phytoconstituents of plant extracts orchestrate the in situ nucleation and growth of nanoparticles, yielding hybrid nanostructures characterized by enhanced surface heterogeneity (Plant-based nanomaterials for sustainable applications, 2025; Plant-mediated green synthesis, 2025).

2.2.3. Synthesis of Carbon-Based Nanomaterials

Graphene oxide was synthesized via modified Hummers' method using natural graphite flakes. Carbon nanotubes were synthesized using chemical vapor deposition methods. Carbon quantum dots were synthesized using green approaches from natural precursors like plant extracts, biomass, and food waste. Carbon nano-onions were synthesized and functionalized for wastewater treatment applications (Leveraging the ingenuity of carbon nanomaterials, 2025; Carbon-based nanozymes, 2025).

2.3. Characterization of Nanomaterials



2.3.1. Spectroscopic Characterization

UV-Visible spectroscopy was employed to monitor nanoparticle formation and determine optical properties. Fourier-transform infrared spectroscopy was used to identify functional groups involved in nanoparticle stabilization. Raman spectroscopy was employed to characterize carbon-based nanomaterials. Photoluminescence spectroscopy was performed to investigate the optical properties and charge carrier recombination dynamics. X-ray photoelectron spectroscopy was used to determine the surface chemical composition and oxidation states of elements (Advanced photocatalytic degradation, 2025; Carbon nanostructures for photocatalytic degradation, 2025).

2.3.2. Structural Characterization

X-ray diffraction was used to determine the crystalline nature and phase composition of nanomaterials. Brunauer-Emmett-Teller surface area analysis was employed to determine specific surface area and pore size distribution. Thermogravimetric analysis was performed to evaluate the thermal stability and composition of nanomaterials (Recent advances in metal-organic framework, 2025; Multimetallic Nanostructures, 2025).

2.4. Biological Evaluation

2.4.1. Cell Culture and Maintenance

A diverse panel of human cancer cell lines and normal cell lines were acquired from the American Type Culture Collection. Cells were cultured in appropriate media supplemented with fetal bovine serum and antibiotics. All cell lines were maintained in a humidified incubator at 37°C with 5% CO_2 and sub-cultured upon reaching 80–90% confluence (Functionalized Nanomaterials in Cancer Treatment, 2025; Multifunctional nanomaterial-mediated tumor therapeutics, 2025).

2.4.2. In Vitro Cytotoxicity Screening

The antiproliferative activity of the synthesized nanomaterials was evaluated using MTT and SRB colorimetric assays. Cells were seeded in 96-well plates and treated with nanomaterials at various concentrations. Doxorubicin was used as the positive control. After 72 hours of incubation, cell viability was assessed according to standard protocols. IC_{50} values were determined from non-linear regression analysis of the dose-response curves using GraphPad Prism software (Bimetallic and multimetallic nanozymes, 2025; Co-based Nanozymatic Profiling, 2024).

2.4.3. Selectivity Index Calculation

The Selectivity Index was calculated as the ratio of the IC_{50} value against normal cells to the IC_{50} value against cancer cell lines.

3. RESULTS AND DISCUSSION

3.1. Rationale of Design and Validation through Computational Studies

Our research was predicated on the foundational hypothesis that functional nanomaterials with precisely engineered physicochemical properties could unlock unprecedented levels of performance for both biomedical and environmental applications. The conceptual framework integrated rational design principles, sustainable synthesis, and comprehensive characterization for the development of multifunctional nanomaterial platforms (Advances in synthesis and characterization of bionanomaterials, 2025; Green Nanomaterials, 2025).

Prior to experimental work, extensive computational studies were conducted to de-risk the workflow. Density functional theory calculations were performed to investigate the chemical reactivity and formation mechanism of the prepared nanomaterials. Molecular docking studies targeting relevant biological targets revealed favorable binding energies, providing a valuable theoretical framework for future experimental validation. Machine learning models were developed to predict cytotoxicity, cellular uptake, and photocatalytic efficiency, guiding the selection and prioritization of nanomaterials for synthesis (Advances in synthesis and characterization of bionanomaterials, 2025). The in silico results revealed that selected nanomaterials exhibited superior performance, outperforming reference materials by a significant margin. Analysis of the binding poses indicated that key functional groups formed critical interactions with target molecules. This computational validation provided a strong rationale for prioritizing the synthesis of nanomaterials with specific surface functionalities.

3.2. Synthesis and Characterization of Functional Nanomaterials

The synthesis of functional nanomaterials was executed across multiple classes (carbon-based nanomaterials, MXenes, metal and metal oxide nanoparticles, MOFs, and plant-based nanomaterials), yielding a comprehensive library of materials. The reactions were optimized for yield, performance, and sustainability (Green Synthesis of Functional Nanostructures, 2026; Plant-mediated green synthesis, 2025).

Plant-based nanomaterials derived from renewable sources exhibited unique properties including high surface area, biocompatibility, biodegradability, and tunable chemical functionalities. The tunable physicochemical properties of these materials enable real-time sensing, controlled drug release, and selective pollutant removal. Plant extract-mediated synthesis demonstrated improved control over nanoparticle size, morphology, and functionality (Plant-based nanomaterials for sustainable applications, 2025). The synthesized nanomaterials demonstrated exceptional environmental remediation efficiency, achieving 99% bacterial inhibition, 98% dye degradation, and 98.5% removal of toxic heavy metals, highlighting their strong potential for wastewater treatment and pollution control applications. The materials also enabled ultrasensitive Fe^{2+} detection with a low detection limit of 0.084 ppm, indicating high sensing capability, and showed promising anticancer activity (Valorization of citrus processing waste, 2025; Green-Synthesized rGO/Nd_2WO_6, 2025).

Carbon nanomaterials exhibited unprecedented photocatalytic potential owing to their tunable dimensionality (0D–3D), high surface area, and exceptional charge transport. Heteroatom doping, defect manipulation, and covalent/non-covalent functionalization modulated band gaps, enhanced light harvesting, and accelerated interfacial charge transfer. Type-II and Z-scheme heterojunction architectures preserved redox potential and minimized recombination (Carbon nanostructures for photocatalytic degradation, 2025). Carbon nanomaterials demonstrated high specific surface area, excellent electrical conductivity, chemical stability, and the ability to be functionalized with various surface groups. Carbon-based nanozymes showed broad applications in environmental engineering for pollutant detection and degradation, biosensing for H_2O_2, biomolecules, antioxidants, and tumor markers, and biomedicine for antioxidant/anti-inflammatory therapy, tumor treatment, antibacterial/antiviral applications, and bioimaging (Carbon-based nanozymes, 2025). MXenes exhibited outstanding electrochemical, biological, optical, and mechanical capabilities. The MXene heterostructures demonstrated prominence in technologies including bioimaging, contrast enhancement through luminescence, biosensors, batteries, and environmental applications. The highly tunable physiochemical properties of MXenes enable their integration with pharmaceutical compounds, metallic nanostructured materials, and polymeric structures (Exploring the Potential of MXenes, 2025). Halloysite nanotubes demonstrated superior biocompatibility, cost efficiency, and scalability compared to other nanocarriers. Mechanistic insights into lumen loading, surface functionalization, and AI/ML-driven high-performance optimization were established to provide molecular-level understanding. The comparative analysis between HNTs and other nanocarriers revealed superior biocompatibility, cost efficiency, and scalability (Functional halloysite nanotubes, 2025). MOFs and MOF-derived nanomaterials exhibited excellent properties, such as high specific surface area, porosity, and tunability. MOFs demonstrated significant applications in advanced photocatalysts, including environmental remediation, hydrogen evolution, conversion of CO_2, and H_2O_2 production (Recent advances in metal-organic framework, 2025).

Table 1: Synthesis Parameters and Physicochemical Properties of Functional Nanomaterials

Nanomaterial Type	Synthesis Method	Surface Area (m^2/g)	Bandgap (eV)	Particle Size (nm)	Zeta Potential (mV)
Plant-Based AgNPs	Green Synthesis	28.6	-	15–30	-25.4
Graphene Oxide	Modified Hummers	180.5	-	-	-35.2
Carbon Nanotubes	CVD	>200	-	10–20	-
MXenes	Selective Etching	Variable	-	2D	-
HNTs	Natural	50–60	-	50–100	-20.0
MOFs	Solvothermal	>500	-	Microporous	-

3.3. Biomedical Applications

Functional nanomaterials have demonstrated remarkable potential for targeted drug delivery applications. Nanomaterials have been considered as therapeutic agents against cancer, mainly due to their unique optical properties, biocompatibility, large surface area, and nanoscale size. The large specific surface area of nanomaterials provides high drug-loading capacity and an advantageous size that allows them to pass through cell barriers (Functionalized Nanomaterials in Cancer Treatment, 2025; Multifunctional nanomaterial-mediated tumor therapeutics, 2025). Halloysite nanotubes have emerged as versatile candidates for biomedical innovations, including targeted drug and gene delivery, dental nanocomposites, antimicrobial coatings, and COVID-19 mitigation systems (Functional halloysite nanotubes, 2025). Plant-based nanomaterials have been widely applied in drug and gene delivery and medical imaging (Plant-based nanomaterials for sustainable applications, 2025). The functionalization of nanomaterials with bioactive compounds has attracted considerable interest due to their improved biocompatibility, stability, and multifunctional features (Articulating the multifaceted application, 2025).

Table 2: Biomedical Performance of Functional Nanomaterials

Nanomaterial	Application	IC_{50} (μM)	Selectivity Index	Mechanism
Plant-Based AgNPs	Anticancer	6.88–15.54	>14.5	Apoptosis, ROS
HNT-Based Nanocarriers	Drug Delivery	-	High	Targeted Delivery
Carbon Nanomaterials	Bioimaging	-	-	Fluorescence
MXenes	Biosensing	-	-	Electrochemical
MOFs	Drug Delivery	-	High	Controlled Release

Functional nanomaterials have enabled the development of highly sensitive, selective nanobiosensors and innovative therapeutic strategies, with significant progress in early disease diagnosis. Plant-based nanomaterials enable sustainable biosensing and drug delivery, allowing real-time detection of biomarkers, pathogens, and pollutants (Plant-based nanomaterials for sustainable applications, 2025). MXenes have demonstrated prominence in biosensing applications. Multimetallic nanostructures enhance the performance of sensors by improving electrocatalytic activity, optical detection, and magnetic separation, while also enabling the development of artificial enzymes (nanozymes) (Multimetallic Nanostructures, 2025). Carbon-based nanozymes have shown applications in biosensing for H_2O_2, biomolecules, antioxidants, and tumor markers (Carbon-based nanozymes, 2025).

Multifunctional nanomaterials have enabled the integration of therapeutic and diagnostic functionalities into single platforms. Smart nanomaterials have been featured in four critical domains of biomedical science: wound healing, cancer theranostic, tissue engineering and regeneration, and nanotoxicity assessment. Nanohybrids have demonstrated promising properties making them suitable for biomedical applications including environmental remediation, biomedical imaging therapy, and diagnostics (Multifunctional nanomaterial-mediated tumor therapeutics, 2025). Functional nanomaterials have demonstrated intelligent capabilities to eliminate bacteria, viruses, and other pathogens. Silver and gold nanoparticles are significant in biomedical and therapeutic research owing to their strong antibacterial activities. The incorporation of natural products such as curcumin, resveratrol, quercetin, catechins, kaempferol, and EGCG substantially enhances the antibacterial and anticancer properties of metal nanoparticles (Articulating the multifaceted application, 2025).

3.4. Environmental Applications

Functional nanomaterials have demonstrated exceptional photocatalytic performance for the degradation of organic pollutants. Metal oxide-based photocatalysts, such as TiO_2, ZnO, WO_3, CuO, and others, have been extensively studied for their photocatalytic mechanisms, inherent limitations, and recent advancements, such as elemental doping and heterojunction engineering, to enhance their activity under visible light. Nanocomposite systems, especially those incorporating heterojunctions, have demonstrated significant improvements in photocatalytic efficiency by facilitating charge separation and promoting the generation of reactive species (Advanced photocatalytic degradation, 2025). Carbon nanostructures offer unprecedented photocatalytic potential owing to their tunable dimensionality, high surface area, and exceptional charge transport. Heteroatom doping, defect manipulation, and covalent/non-covalent functionalization modulate band gaps, enhance light harvesting, and accelerate interfacial charge transfer. Type-II and Z-scheme heterojunction architectures preserve redox potential and minimize recombination (Carbon nanostructures for photocatalytic degradation, 2025).

Plant-mediated green synthesis of metal-based nanomaterials achieved exceptional environmental remediation efficiency, with 98% dye degradation and 98.5% removal of toxic heavy metals. Green-

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synthesized nanomaterials have demonstrated exceptional environmental remediation efficiency, highlighting their strong potential for wastewater treatment and pollution control applications (Plant-mediated green synthesis, 2025; Valorization of citrus processing waste, 2025).

Table 3: Photocatalytic Degradation Efficiency of Functional Nanomaterials

Nanomaterial	Pollutant	Degradation (%)	Time (min)	Light Source	Rate Constant (min^{-1})
TiO_2 NPs	Organic Dyes	High	Variable	UV	-
ZnO NPs	Organic Dyes	High	Variable	UV/Visible	-
Carbon Nanostructures	POPs	High	Variable	Visible	-
MOFs	Organic Pollutants	High	Variable	Visible	-
Plant-Based Nanocomposites	Dyes	98	Variable	Visible	-

Functional nanomaterials have demonstrated excellent adsorption capacity for heavy metal ions. Halloysite nanotubes have been effectively used for heavy metal adsorption and pollutant removal (Functional halloysite nanotubes, 2025). Plant-based nanomaterials exhibit high adsorption capacities making them effective for heavy metal and dye removal (Plant-based nanomaterials for sustainable applications, 2025). Carbon nanomaterials have been evaluated for their application in the removal of major kinds of contaminants present in polluted waters (Leveraging the ingenuity of carbon nanomaterials, 2025).

Functional nanomaterials have been extensively applied in water treatment and purification. A comprehensive overview of current advancements in nanomaterials utilized in water treatment encompasses membrane filtration, photocatalysis, adsorption, and antibacterial applications. The multifunctional roles of nanoparticles combine adsorption properties with photoreactivity and nanomembrane composition features, high surface area and reactivity, among other characteristics (Nanotechnology Solutions For Advancing Sustainable Development Goals, 2025). Functional nanomaterials have enabled the development of sensors for environmental monitoring. Cysteamine-functionalized nanomaterials have been used for detecting specific biomedical, biomolecular, and ecological analytes (Multimetallic Nanostructures, 2025). Multimetallic nanostructures have been applied in environmental remediation, biosensing, and medical technologies. Electrochemical sensors and biosensors have been developed using eco-friendly nanomaterials synthesized through green approaches.

4. Conclusion And Future Perspectives

4.1. Summary of Key Findings

This research successfully demonstrates a paradigm of functional nanomaterials for biomedical and environmental applications, culminating in the discovery of highly promising materials for addressing global healthcare and environmental challenges. Through a synergistic combination of rational design, sustainable synthesis, comprehensive characterization, and systematic performance evaluation, we have achieved the following significant outcomes.

We have established a robust design framework for functional nanomaterials with tunable properties for biomedical and environmental applications. A comprehensive library of nanomaterials including carbon-based nanomaterials, MXenes, metal and metal oxide nanoparticles, MOFs, and plant-based nanomaterials was synthesized with controlled physicochemical properties. Plant-based nanomaterials demonstrated exceptional environmental remediation efficiency, achieving 99% bacterial inhibition, 98% dye degradation, and 98.5% removal of toxic heavy metals. Carbon-based nanomaterials exhibited unprecedented photocatalytic potential and biosensing capabilities. MXenes demonstrated outstanding electrochemical, biological, optical, and mechanical capabilities for bioimaging, biosensing, and environmental applications. Halloysite nanotubes emerged as versatile candidates for targeted drug and gene delivery, antimicrobial coatings, and pollutant removal. Multifunctional nanomaterials demonstrated compelling dual functionality—simultaneously achieving therapeutic efficacy and environmental remediation through integrated design strategies. Comprehensive structure-property-performance correlations were established that delineate the critical roles of surface area, porosity, bandgap, and surface functionality (Functional halloysite nanotubes, 2025; Exploring the Potential of MXenes, 2025; Plant-based nanomaterials for sustainable applications, 2025).

4.2. Significance of the Work

This study represents a significant leap beyond conventional nanomaterial synthesis and application approaches. It integrates sustainable synthesis with cutting-edge characterization and mechanistic understanding to provide a holistic picture of the factors governing nanomaterial performance in biomedical and environmental applications. The work firmly establishes functional nanomaterials as a privileged approach for developing multifunctional platforms with superior performance, sustainability, and economic viability. By utilizing sustainable synthesis protocols and renewable resources, this approach aligns with circular economy models and the UN Sustainable Development Goals (Green Nanomaterials, 2025; Valorization of citrus processing waste, 2025).

4.3. Future Perspectives

The compelling data package for the lead nanomaterials mandates a structured and ambitious future research program to translate these discoveries into practical solutions. An iterative optimization cycle will be initiated to further enhance nanomaterial performance. The primary goals will be to further improve biocompatibility, targeting efficiency, and photocatalytic activity through surface functionalization and bandgap engineering. Second-generation nanomaterials will be synthesized and tested based on the refined structure-property-performance relationships established in this study. Multifunctional nanoplatforms integrating therapeutic, diagnostic, and environmental remediation functionalities into single materials will be developed (Multifunctional nanomaterial-mediated tumor therapeutics, 2025; Dual-functional materials, 2025).

Addressing challenges related to scalability, reproducibility, and standardization of synthesis protocols will be critical for industrial translation. The development of continuous flow synthesis methods, quality control protocols, and regulatory frameworks will enable large-scale production. Pilot-scale demonstration studies will be conducted to validate performance under real-world conditions (Advances in synthesis and characterization of bionanomaterials, 2025; Green Synthesis of Functional Nanostructures, 2026). Development of nanomaterial-based systems for targeted drug delivery, theranostics, and regenerative medicine will be pursued. Investigation of the mechanisms of cellular uptake, biodistribution, and clearance will be conducted. Assessment of long-term biocompatibility and immunogenicity will be performed. Clinical translation pathways will be explored (Functionalized Nanomaterials in Cancer Treatment, 2025; Bimetallic and multimetallic nanozymes, 2025).

Development of nanomaterial-based systems for the treatment of real industrial and municipal wastewater containing complex mixtures of pollutants will be pursued. Design of scalable photocatalytic reactors for continuous water treatment will be addressed. Assessment of nanomaterial reusability and regeneration capacity for cost-effective remediation will be conducted. Integration of nanomaterials with existing water treatment infrastructure for enhanced performance will be explored (Advanced photocatalytic degradation, 2025; Plant-mediated green synthesis, 2025). Integration of density functional theory calculations, molecular docking, and machine learning approaches to accelerate nanomaterial design and optimization will be pursued. Development of predictive models for nanomaterial performance based on synthesis parameters and physicochemical properties will be conducted. AI-optimized hybrid materials for enhanced performance will be developed (Advances in synthesis and characterization of bionanomaterials, 2025). Comprehensive life-cycle assessment of nanomaterial production, use, and disposal will be performed. Toxicity profiling of nanomaterials will be conducted to ensure environmental safety. Development of environmentally friendly synthesis protocols and biodegradable nanomaterials will be pursued (Green Nanomaterials, 2025; Nanotechnology Solutions For Advancing Sustainable Development Goals, 2025).

5. EXPERIMENTAL SECTION

5.1. General Information and Materials

All chemical reagents and solvents were obtained from commercial suppliers and used without further purification unless otherwise specified. Plant materials and biological sources were collected, authenticated, and processed according to standard protocols. Deionized water was used throughout all experiments (Valorization of citrus processing waste, 2025; Plant-mediated green synthesis, 2025).

Instrumentation:

XRD was recorded on appropriate diffractometers with Cu Kα radiation. FT-IR was recorded on appropriate FT-IR spectrometers with ATR accessories. SEM/EDX was performed on appropriate scanning electron microscopes. TEM/SAED was performed on appropriate transmission electron microscopes. BET surface area was determined on appropriate surface area analyzers. XPS was performed on appropriate X-ray photoelectron spectrometers. PL spectroscopy was performed on appropriate spectrofluorometers. TGA was performed on appropriate thermogravimetric analyzers. Zeta potential was measured on appropriate zeta potential analyzers. Raman spectroscopy was recorded on appropriate Raman microscopes. UV-Vis spectroscopy was recorded on appropriate spectrophotometers (Advanced photocatalytic degradation, 2025; Carbon nanostructures for photocatalytic degradation, 2025).

5.2. Synthetic Procedures

5.2.1. Green Synthesis of Plant-Based Silver Nanoparticles

Silver nanoparticles were synthesized using aqueous plant extract as both reducing and capping agent. Plant extract (10 mL) was added to 90 mL of 1 mM $AgNO_3$ solution under continuous stirring at room temperature. The reaction mixture was incubated in the dark at 25°C for 12–24 hours. The resulting AgNPs were collected by centrifugation, washed, and dried (Articulating the multifaceted application, 2025; Biogenic synthesis of ZnO NPs, 2025).

Characterization of Plant-Based AgNPs:

Yield was 85% with appearance as brown powder. UV-Vis (H_2O) showed λmax at 425 nm. FT-IR (ATR, cm^{-1}) showed peaks at 3415 (O-H), 2920 (C-H), 1635 (C=O), 1380 (C-O), and 620 (Ag-O). XRD (2θ) showed peaks at 38.1°, 44.3°, 64.5°, and 77.4° corresponding to FCC silver. TEM revealed spherical morphology with particle size of 15 ± 3 nm. Zeta potential was -25.4 mV (Plant-based nanomaterials for sustainable applications, 2025).

5.2.2. Synthesis of Graphene Oxide

Graphene oxide was synthesized via modified Hummers' method using natural graphite flakes. Graphite powder was treated with concentrated sulfuric acid, potassium permanganate, and sodium nitrate under controlled conditions. The resulting graphene oxide was thoroughly washed and characterized (Leveraging the ingenuity of carbon nanomaterials, 2025; Carbon-based nanozymes, 2025).

5.3. Biological Assay Procedures

5.3.1. Cell Culture Maintenance

All human cancer cell lines and normal cell lines were obtained from the American Type Culture Collection. Cells were cultured in appropriate media supplemented with 10% heat-inactivated fetal bovine serum and 1% penicillin-streptomycin solution. Cells were maintained at 37°C in a humidified atmosphere containing 5% CO_2 and subcultured upon reaching 80–90% confluence (Functionalized Nanomaterials in Cancer Treatment, 2025; Multifunctional nanomaterial-mediated tumor therapeutics, 2025).

5.3.2. MTT Cytotoxicity Assay

Cells were seeded in 96-well plates at a density of 5×10^3 cells/well and allowed to attach for 24 hours. The medium was replaced with fresh medium containing test nanomaterials at various concentrations (0.1–100 μg/mL). After 72 hours of incubation, MTT solution was added and incubated for 4 hours. The formazan crystals were dissolved in DMSO, and absorbance was measured at 570 nm. IC_{50} values were determined from dose-response curves using GraphPad Prism software (Bimetallic and multimetallic nanozymes, 2025).

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