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Multifunctional Nanomaterials in Materials Chemistry: A Cross-Disciplinary Review of Applications in Energy, Environment, Catalysis, and Biomedicine

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Abstract

Review Article

Multifunctional nanomaterials are at the frontier of materials chemistry, having the ability to allow customised property and structure-integrated functionalities to facilitate various applications in energy conversion, environmental remediation, catalysis, biomedical systems and chemical sensing. With sophisticated control of composition, morphology and surface chemistry, extensive families of nanostructures have been designed that satisfy the requirements of a particular application, including metal and metal oxide nanoparticles, carbon-based materials (e.g. graphene and carbon nanotubes), metalorganic frameworks, perovskite materials and hybrid nanocomposites. This familiarization is a critical assessment of recent progress in their synthesis, structure--function relationships and performance of applicability across various disciplines. In spite of the changes that have been achieved, there are still a number of challenges that have not been dealt with. These are gaps in mass manufacturing, lack of long-term stability in its functioning, and combination of numerous functionalities in one system, and toxicity, biodegradability and persistence issues. Responding to these issues, the review proposes the following key future directions, namely sustainable and green synthesis methodologies, machine learning to predict and optimize materials, design of bioinspired multifunctional systems, and standardization of safety and regulatory assessment. This brings together three fields chemistry, nanotechnology, and materials engineering to present a comprehensive view on how to develop and implement next-generation nanomaterials to have a cross-sectoral influence.

Keywords: Multifunctional, nanomaterials, Materials, chemistry, Nanostructured, materials, Environmental, remediation Catalysis, Energy, storage and conversion, Drug delivery Chemical sensing Hybrid nanocomposites Green synthesis.

1. INTRODUCTION

Multifunctional nanomaterials (MFNMs) are an emerging class of nanoscale materials engineered to exhibit multiple, often synergistic, functions within a single structural unit. These multifunctional capabilities arise from the deliberate combination of physical, chemical, optical, magnetic, or biological properties, enabling a broad spectrum of applications across disciplines such as medicine, energy, agriculture, and materials science. Typically, MFNMs are constructed by integrating two or more distinct material types—such as metals, ceramics, polymers, or biomolecules—into a

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nanostructure, resulting in enhanced or entirely new functionalities (Wu *et al.,* 2018; Wang *et al.,* 2019; Freund *et al.,* 2018). Their hallmark lies in the capacity to integrate varied functionalities within one architecture, which allows for dual or multiple actions. In biomedical applications, for instance, a single MFNM may enable both imaging and targeted drug delivery. Similarly, in energy systems, MFNMs may simultaneously enhance energy storage, conversion, and catalytic efficiency (Yáñez-Sedeño *et al.,* 2020; Sadiq *et al.,* 2023). The design and realization of these materials typically involve strategies like core–shell architectures, hybrid composites, and surface modifications.

The historical emergence of MFNMs is closely tied to advances in nanotechnology and materials science toward the end of the 20th century. Initially, nanomaterials were developed with a single intended function—such as improving mechanical strength or catalysis. However, as scientific and industrial challenges became more complex and interdependent, there was a shift toward materials that could address multiple problems simultaneously. The growth of interdisciplinary research and the development of more precise fabrication techniques—such as microfluidic systems, solvothermal synthesis, and click chemistry—enabled the synthesis of nanostructures with integrated functionalities (Yuan *et al.,* 2017; Wu *et al.,* 2024). In the past decade, MFNMs have gained substantial research attention due to their versatility and ability to meet the demands of fields like personalized medicine, green energy, and environmental remediation. With an improved understanding of nanoscale interfacial interactions, researchers now harness the synergistic effects that arise when multiple components function together in ways not achievable when used independently (Prakash, 2016; Wang *et al.,* 2019).

Within materials chemistry, MFNMs mark a transformative shift in material design philosophy. Their tailored size, morphology, and surface chemistry offer a high degree of control over their physicochemical properties. MFNMs are central to developing next-generation materials that exceed the performance capabilities of traditional substances, especially in areas like catalytic efficiency, optical behavior, electrical conductivity, and mechanical durability (Freund *et al.,* 2018; Wu *et al.,* 2024). For example, in catalysis, MFNMs have been used to design nanocatalysts that simultaneously facilitate chemical reactions and remove environmental pollutants. In the biomedical arena, MFNMs have enabled the creation of smart drug delivery systems capable of imaging tumors, targeting therapy, and monitoring treatment responses using a single platform (Srinath *et al.,* 2023; Aires *et al.,* 2020). Their significant role in materials chemistry arises from their ability to bridge the gap between fundamental chemical principles and real-world applications, pushing the discipline toward intelligent and sustainable technologies.

Multifunctional nanomaterials also exemplify the interdisciplinary nature of contemporary scientific research. Their development draws upon concepts and techniques from chemistry, physics, materials science, biology, engineering, and medicine. For example, in biomedicine, MFNMs enable "theranostics"—a fusion of therapy and diagnostics in one system (Sadiq *et al.,* 2023; Wu *et al.,* 2018). In energy science, they contribute to the performance of supercapacitors, lithium-ion batteries, and fuel cells by enhancing charge transfer, durability, and overall system efficiency (Wu *et al.,* 2024; Wang *et al.,* 2019). In agriculture, MFNMs are being employed in the controlled delivery of agrochemicals, soil health monitoring, and real-time pathogen detection (Abd-Elsalam, 2020). Environmental applications include pollutant degradation, water purification, and contaminant sensing, often in extreme or hostile settings (Wu *et al.,* 2018; Freund *et al.,* 2018). The design and deployment of these materials are typically the result of collaborative efforts that integrate knowledge from synthetic chemists, materials engineers, environmental scientists, and medical researchers—further illustrating their cross-disciplinary significance.

This review focuses on the design, synthesis, and applications of MFNMs reported between 2016 and 2025. Studies selected for discussion adhere to a rigorous set of criteria, including publication in peer-reviewed journals and emphasis on multifunctionality—defined as the integration of two or more distinct properties such as catalytic-optical, magnetic-therapeutic, or electrochemical-sensing functions. Applications are examined in diverse domains such as biomedicine, renewable energy, sustainable agriculture, and environmental remediation. In addition, the review discusses core design methodologies, such as core–shell structures, hybrid nanocomposites, and surface functionalization techniques. Central to the scope of this review is also the critical evaluation of key challenges that limit real-world implementation. These include issues of synthesis complexity, economic scalability, and reproducibility. Recent computational advances, particularly in density functional theory (DFT), have further expanded the design possibilities for multifunctional materials by enabling accurate predictions of their structural, electronic, optical, and thermoelectric properties before experimental synthesis. For example, Nazar *et al.,* (2025) employed DFT and BoltzTraP2 calculations to investigate the halide double perovskites Rb_2TlSbX_6 (X = Cl, Br, I) for solar cell applications, revealing their dynamic and thermodynamic stability through phonon dispersion analysis and the absence of imaginary frequencies. Their work demonstrated how compositional tuning in perovskite frameworks can yield favorable optoelectronic band structures, mechanical robustness, and promising thermoelectric performance. Such computational insights not only accelerate the discovery of high-performance, multifunctional materials but also provide a rational basis for tailoring their properties toward targeted energy conversion and green technology applications.

Despite impressive scientific progress, several critical research gaps persist in the field of MFNMs. Scalability remains a major hurdle. While laboratory-scale synthesis of MFNMs has been demonstrated with high functional precision, transitioning these methods to industrial-scale production is far from straightforward. Technologies such as microfluidic reactors offer potential but require substantial optimization for continuous and cost-effective manufacturing (Wu *et al.,* 2024; Yuan *et al.,* 2017). Another major limitation is long-term functionality, particularly in real-world conditions. MFNMs can suffer from structural instability due to oxidation, aggregation, or degradation, which reduces their efficiency in both biomedical and energy applications over time (Sadiq *et al.,* 2023; Srinath *et al.,* 2023). Reproducibility is also a concern; minor variations in precursor composition, environmental factors, or synthesis parameters can significantly affect material properties and performance (Freund *et al.,* 2018; Prakash, 2016). Furthermore, the biocompatibility and toxicity profiles of MFNMs remain incompletely understood. As multifunctionality often involves complex coatings, ligands, or doping agents, these additions may introduce unforeseen toxicological effects, especially in clinical applications (Aires *et al.,* 2020; Sadiq *et al.,* 2023). Another technical barrier is functional interference, where multiple active components embedded within the same structure may hinder rather than enhance each other's performance. For example, magnetic components may dampen optical signals, compromising multifunctionality (Wu *et al.,* 2018).

In summary, multifunctional nanomaterials represent a paradigm shift in materials science, enabling multifunctionality within a singular platform to address complex and interdisciplinary challenges. While they offer significant promise across sectors including medicine, energy, and the environment, future research must address the persistent limitations related to scalability, long-term performance, and safe integration into practical systems.

2. Classification of Multifunctional Nanomaterials

2.1. Metal and Metal Oxide Nanoparticles (e.g., Ag, ZnO, TiO_2)

Metal and metal oxide nanoparticles (MONPs) are foundational to the development of multifunctional nanomaterials due to their unique structural properties and diverse functional behaviors. Typically synthesized within the size range of 5 to 150 nm, these nanoparticles exhibit enhanced surface-to-volume ratios and reactive surfaces, which facilitate interactions with light, biological systems, and chemical targets. For example, silver (Ag) nanoparticles commonly measure between 50–100 nm, while zinc oxide (ZnO) and titanium dioxide (TiO_2) particles range from 16–120 nm, depending on synthesis methods such as sol-gel, hydrothermal, or co-precipitation techniques (Anandaraj & Ilakkiya, 2018; Jeyashanthi *et al.,* 2016). The intrinsic crystallinity and morphology of these particles play a vital role in determining their functionality. ZnO nanoparticles, for instance, often exhibit wurtzite crystal structures with surface defects and oxygen vacancies, which enhance reactive oxygen species (ROS) generation—a key mechanism in antimicrobial and photocatalytic activity (Sharma *et al.,* 2020). TiO_2 typically appears in anatase or rutile phases and is known for its wide bandgap and strong UV absorption, both critical for effective photocatalysis (Amiri *et al.,* 2022).

To further tailor their properties, strategies such as doping, alloying, and composite formation are employed. Doping, particularly with Ag, enhances visible light absorption and increases antimicrobial or catalytic efficiency by introducing surface plasmon resonance (SPR) effects. For instance, Ag-doped ZnO has shown improved antibacterial and optical properties compared to its undoped counterpart (Anbarasu *et al.,* 2024). Core–shell nanostructures such as Ag@ZnO or TiO_2@Ag leverage synergistic interactions between the core and shell materials, enhancing stability, reactivity, and multifunctionality. Such heterostructures demonstrate combined effects such as enhanced photocatalytic degradation and targeted pathogen inactivation, with ZnO/TiO_2 arrays achieving up to 99% bacteriostatic efficiency while maintaining cytocompatibility (Pang *et al.,* 2019). Additionally, surface functionalization using organic molecules like citrate, chitosan, or natural plant extracts significantly enhances colloidal stability and biocompatibility while improving interaction with microbial membranes or environmental pollutants (Alavi & Nokhodchi, 2021).

Green synthesis techniques have also emerged as sustainable alternatives, using biological agents such as plants and microbes to produce nanoparticles under eco-friendly conditions. For instance, ZnO nanoparticles synthesized using *Tithonia diversifolia* extracts yielded particles around 20 nm in size with notable antibacterial properties, demonstrating the potential of green routes in biomedical and environmental applications (Wafula *et al.,* 2020).

The multifunctional nature of MONPs supports a wide range of applications. In biomedicine, Ag, ZnO, and TiO_2 nanoparticles are used for their ROS-generating abilities, membrane-disruptive effects, and photo-activated therapeutic functionalities. ZnO/Ag composites have effectively inhibited *E. coli* and other pathogens, serving as promising antibiotic alternatives (Sharma *et al.,* 2020). Furthermore, TiO_2-ZnO coatings on orthopedic implants not only prevent bacterial colonization but also support bone tissue regeneration (Pang *et al.,* 2019). Environmental remediation is another critical area where these nanoparticles shine. Photocatalytic systems composed of ZnO and TiO_2

degrade organic pollutants and dyes effectively under sunlight due to optimal bandgap alignment and efficient charge separation, with up to 78% degradation observed in some systems (Vijayalakshmi & Asvini, 2018; Butola *et al.,* 2018).

In the textile and coating industry, MONPs are integrated into smart fabrics to impart properties such as UV resistance, self-cleaning, and antimicrobial activity. For example, cotton fabrics treated with ZnO and TiO_2 nanoparticles achieve ultraviolet protection factor (UPF) ratings exceeding 50+, while maintaining antibacterial performance even after multiple washes (Kara *et al.,* 2024; Ibrahim *et al.,* 2018). In the field of sensing and diagnostics, ZnO and Ag nanoparticles are utilized in biosensors due to their superior electron transport and surface reactivity. These materials are effective in glucose sensing, gas detection, and environmental pollutant monitoring, making them valuable tools for real-time diagnostics and environmental surveillance (Wang *et al.,* 2019).

Despite these promising applications, several limitations hinder the widespread deployment of multifunctional MONPs. Scalability remains a major challenge; while green and chemical synthesis routes produce high-quality nanoparticles at the laboratory scale, consistent large-scale production remains difficult due to issues in yield and uniformity (Wafula *et al.,* 2020). Reproducibility is also problematic, as minor changes in synthesis conditions such as temperature, pH, and dopant levels can lead to significant variations in nanoparticle morphology and performance (Anandaraj & Ilakkiya, 2018). Environmental concerns are another pressing issue, particularly the toxicity of Ag and ZnO nanoparticles to aquatic ecosystems. Studies have shown that chronic exposure can disrupt microbial populations and affect hematological and gene expression profiles in aquatic organisms such as zebrafish (Anbarasu *et al.,* 2024).

Biocompatibility also warrants caution. While surface functionalization helps mitigate toxicity, high concentrations or prolonged exposure to nanoparticles may lead to excessive ROS accumulation, causing cytotoxicity and inflammation in mammalian cells (Poon *et al.,* 2017). Additionally, functional interference is an emerging concern; efforts to integrate multiple functionalities into a single nanoparticle often result in performance trade-offs. For example, surface coatings intended to improve biocompatibility might block active catalytic or antimicrobial sites, diminishing overall effectiveness (Freund *et al.,* 2018). Addressing these limitations is essential for the safe and effective application of multifunctional MONPs across various industries and environmental systems.

2.2. Carbon-Based Nanomaterials (e.g., Graphene, CNTs, CQDs)

Carbon-based nanomaterials (CBNs) represent a highly versatile and extensively researched category of multifunctional nanostructures, encompassing graphene, carbon nanotubes (CNTs), and carbon quantum dots (CQDs). These materials derive their multifunctional behavior from the ability of carbon atoms to form diverse hybridized structures (sp^2 and sp^3), resulting in zero-dimensional (0D), one-dimensional (1D), and two-dimensional (2D) architectures. Graphene, consisting of a single atomic layer of carbon atoms arranged in a two-dimensional honeycomb lattice, is particularly noted for its extraordinary thermal conductivity, high mechanical strength, and exceptional electronic mobility (Teradal & Jelinek, 2017; Yücer *et al.,* 2025). Carbon nanotubes, which are seamless cylindrical rolls of graphene sheets, possess remarkable tensile strength and electrical conductivity, as well as high aspect ratios that make them favorable for biosensing and drug delivery applications (Gaur *et al.,* 2021; Yücer *et al.,* 2025). Carbon quantum dots and graphene quantum dots, on the other hand, are zero-dimensional materials with diameters typically less than 10 nm. These quantum dots are renowned for their tunable fluorescence, biocompatibility, and high surface area, making them ideal candidates for biomedical imaging, photodynamic therapy, and drug delivery (Asil & Narayan, 2024; Hatta *et al.,* 2023).

The multifunctionality of CBNs is intricately linked to their structural configurations. Graphene's two-dimensional structure allows for a large surface area and superior electron mobility, making it ideal for applications such as biosensors and electronic circuits. CNTs, with their one-dimensional hollow tubular structure, provide unique channels for molecular transport and possess mechanical flexibility, lending themselves to use in wearable electronics and tissue engineering. CQDs, due to their nanoscale size, demonstrate deep tissue penetration and are rapidly cleared by renal systems, enhancing their suitability for in vivo imaging. Their photoluminescence can be fine-tuned by adjusting size, surface passivation, or the incorporation of specific functional groups—a feature governed by quantum confinement and edge effects (Medeiros & Naccache, 2020; Pandey & Chusuei, 2021).

Various engineering strategies have been implemented to further enhance the multifunctional capabilities of CBNs. One common approach is doping, where heteroatoms such as nitrogen, sulfur, or boron are introduced into the carbon framework to alter electronic and optical properties. For instance, nitrogen-doped graphene and CQDs exhibit improved electron transfer rates and stronger photoluminescence, which are advantageous in sensing and therapeutic applications (Asil & Narayan, 2024; ElMorsy *et al.,* 2024). Surface functionalization is another crucial strategy, involving either covalent or non-covalent attachment of drugs, ligands, or biomolecules to enhance dispersion, target specificity, and biocompatibility. Amino-functionalized graphene, for example, has been shown to improve biosensor performance and cellular uptake (Brndiarova *et al.,* 2019). Additionally, the development of core–shell nanostructures, in which carbon-based materials are used as either the core or the shell, enables integrated functionalities such as simultaneous imaging and drug delivery. For example, graphitic carbon nitride quantum dots embedded in carbon nanosheets have demonstrated pH-responsive drug release and near-infrared imaging capabilities (Liu *et al.,* 2020).

These advanced nanostructures have found wide-ranging applications across several disciplines. In biomedicine, graphene and CNTs have been explored for their roles in tissue scaffolding, targeted drug delivery, and neural repair due to their excellent mechanical properties and cellular compatibility (Yücer *et al.,* 2025; Asil *et al.,* 2023). In cancer therapy, CQDs and GQDs act as fluorescent imaging probes and photosensitizers in photodynamic therapy, providing targeted and less invasive treatment options (Ahmed & Abusalah, 2024; Asil *et al.,* 2023). CBNs have also revolutionized the field of biosensing. Their high electrical conductivity and large surface area enable ultra-sensitive detection of biomarkers in electrochemical biosensors (Pandey & Chusuei, 2021). In optoelectronics, CQDs are used in the fabrication of cost-effective, flexible photodetectors and field-effect transistors, contributing to the next generation of wearable and portable electronic devices (Selamneni *et al.,* 2021).

Despite their promising capabilities, the development and deployment of carbon-based nanomaterials face several critical challenges. One major limitation is the difficulty in controlling morphology and size distribution during synthesis, often resulting in heterogeneous samples with inconsistent performance. Additionally, surface reactivity and functionalization reproducibility remain problematic. Non-uniform modification can significantly affect bioavailability and regulatory acceptance, especially for medical applications (Liu *et al.,* 2023). Another pressing issue concerns the long-term biocompatibility and clearance of these materials. While CQDs have demonstrated low toxicity in short-term studies, their behavior in vivo over extended periods remains insufficiently understood and necessitates further investigation (Asil & Narayan, 2024). Furthermore, large-scale production of defect-free, high-purity graphene and CNTs continues to be expensive and technically challenging, limiting their industrial scalability and performance reliability.

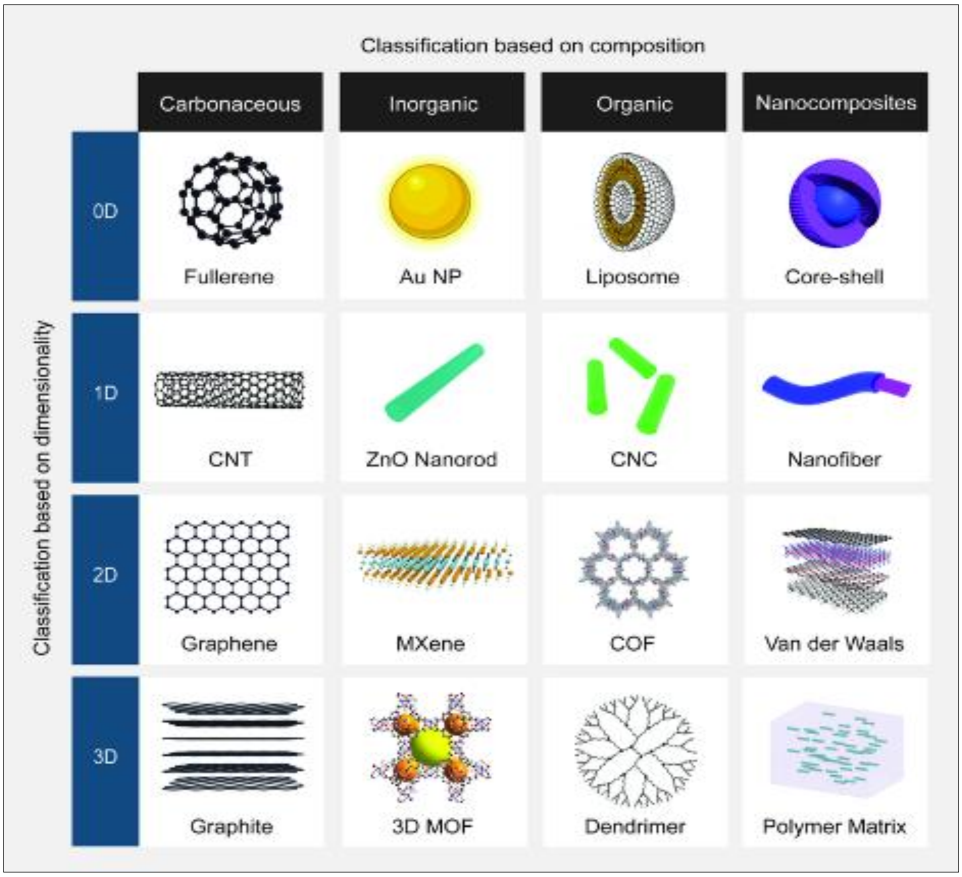

Figure 1: Structures of carbon-based nanomaterials

In conclusion, carbon-based nanomaterials—including graphene, carbon nanotubes, and carbon quantum dots—hold significant promise in the field of multifunctional nanotechnology due to their distinctive structure–property relationships and adaptable surface chemistries. Their integration into biomedical, electronic, environmental, and energy-related applications continues to expand as research overcomes barriers related to synthesis, reproducibility, and long-term safety. Advancing the fundamental understanding of these materials and improving their scalable production will be essential to fully realize their potential in clinical and industrial settings.

An overview of different carbon nanostructures—including graphene sheets, carbon nanotubes, and carbon quantum dots—emphasizing how morphology dictates properties. It captures the diversity in dimensionality (2D–0D) and their capacity to combine electrical, optical, and mechanical functionalities.

2.3. Polymeric Nanostructures and Nanogels

Polymeric nanostructures and nanogels are a subclass of multifunctional nanomaterials composed primarily of synthetic or natural polymers. Their structural diversity and responsiveness to environmental stimuli make them highly attractive for biomedical, pharmaceutical, and environmental applications. These systems include nanogels, micelles, dendrimers, star-shaped polymers, and polymer-coated hybrid nanoparticles. Nanogels are typically 3D crosslinked hydrophilic polymer networks with diameters ranging from 20 to 200 nm, capable of swelling in aqueous media without dissolving. Their porous network structure allows for high loading capacity and controlled release of therapeutic agents, proteins, or imaging molecules (Haque *et al.,* 2021; Zhou *et al.,* 2021). Micelles and polymer somes are self-assembled amphiphilic polymer systems. While micelles have a hydrophobic core useful for drug encapsulation, polymer somes mimic lipid bilayer vesicles and allow dual drug encapsulation in both core and shell compartments (Akhtar *et al.,* 2023).

The functionality of polymeric nanostructures is intrinsically linked to their molecular architecture, crosslinking density, hydrophilic-hydrophobic balance, and surface chemistry. Nanogels exhibit high water content, tunable porosity, and reversible volume changes in response to pH, temperature, or redox conditions. These properties allow for smart drug delivery systems that respond to tumor microenvironments or intracellular triggers (Singh *et al.,* 2023). Dendrimers possess a branched, tree-like structure that enables multivalent functionalization on their periphery, ideal for attaching targeting ligands, drugs, or imaging probes (Li *et al.,* 2021). Amphiphilic copolymers can self-assemble into nanostructures with core–shell morphology, allowing separation of hydrophobic and hydrophilic drugs and enhanced circulation times in vivo (Amina *et al.,* 2024). The degree of crosslinking in nanogels can also modulate their mechanical stability, swelling behavior, and diffusion properties, which directly influence their therapeutic performance and stability in biological environments (Praveen *et al.,* 2024).

Multifunctionality in polymeric nanostructures is achieved through several design strategies. Polymers such as poly(N-isopropylacrylamide) (PNIPAM), polyethylene glycol (PEG), and polyacrylic acid (PAA) are frequently used to build nanogels that respond to stimuli like pH, temperature, or redox potential. For example, dual pH–temperature responsive nanogels can trigger drug release only in acidic tumor environments above body temperature (Haque *et al.,* 2021). Targeting ligands such as folic acid and antibodies, imaging dyes like fluorescein and rhodamine, or antimicrobial agents such as silver nanoparticles can be conjugated onto the nanogel or micelle surface, enabling diagnostic and therapeutic integration (Amina *et al.,* 2024; Akhtar *et al.,* 2023). Hydrophobic drugs can be encapsulated within micelle cores, while hydrophilic agents reside in nanogel matrices or polymer some interiors. Dual drug-loading strategies have shown synergistic therapeutic effects, especially in cancer therapy (Singh *et al.,* 2023). Additionally, polymeric nanostructures can be hybridized with inorganic materials like gold nanoparticles, iron oxide, or quantum dots. These hybrids exhibit combined imaging, magnetic targeting, and drug delivery properties, increasing their utility in precision medicine (Praveen *et al.,* 2024).

The biomedical relevance of these systems is extensive. Nanogels and micelles have been extensively studied for cancer therapy due to their controlled release behavior and ability to protect sensitive drugs like proteins or nucleic acids. pH-responsive nanogels have been successfully used for delivery of doxorubicin, achieving enhanced cytotoxicity in acidic tumor environments (Haque *et al.,* 2021; Singh *et al.,* 2023). Polymeric nanostructures functionalized with fluorescent dyes or nanoparticles enable in vivo imaging and real-time tracking. For instance, rhodamine-labeled nanogels have shown strong tumor accumulation and fluorescence signals in preclinical imaging studies (Zhou *et al.,* 2021). Moreover, polymeric nanogels loaded with silver or cationic polymers exhibit strong antimicrobial activity against multi-drug-resistant strains. Thermo-responsive hydrogels have been used in wound dressings to provide on-demand drug release and improve healing outcomes (Amina *et al.,* 2024). Dendritic polymers and cationic nanogels have shown excellent capacity for encapsulating and protecting siRNA and plasmid DNA, facilitating efficient transfection and gene silencing with minimal cytotoxicity (Li *et al.,* 2021).

Despite significant progress, several challenges remain in the development and translation of polymeric nanostructures. Reproducibility and scalability are significant issues; batch-to-batch variation in polymer synthesis, crosslinking, and self-assembly results in inconsistent particle sizes and drug release kinetics, complicating clinical translation (Praveen *et al.,* 2024). Long-term stability is another concern, as many nanogels undergo aggregation or degradation in biological fluids, limiting shelf-life and delivery efficiency. Additionally, biodegradability remains a key hurdle—some synthetic polymers, particularly those with dense crosslinking, are not easily metabolized or excreted, raising concerns about long-term toxicity. Regulatory barriers further complicate development, as multifunctional systems with hybrid compositions face uncertainty in classification as drugs, devices, or combination products (Akhtar *et al.,* 2023). Finally, while in vitro studies are abundant, there is a notable lack of comprehensive in vivo pharmacokinetics, toxicity, and immunogenicity data for most nanogel formulations, hindering their clinical advancement.

3. Nanomaterials in Energy Applications

3.1. Photovoltaics and Perovskite Solar Cells

Figure 2 illustrates the architecture of tandem perovskite solar cells integrating a perovskite top cell and a bottom cell made from materials such as silicon (Si), copper indium gallium selenide (CIGS), or organic semiconductors. This layered design demonstrates how nanostructuring strategies are employed to maximize light absorption, optimize charge carrier dynamics, and improve overall device performance. The diagram also highlights the importance of compositional tuning and interfacial engineering, which are critical in advancing perovskite-based photovoltaic systems.

Perovskite solar cells have emerged as one of the most promising next-generation photovoltaic technologies due to their high power conversion efficiencies, tunable bandgaps, and relatively low fabrication costs. Since their introduction in 2009, where the initial efficiencies were only around 3.8%, continuous development in materials chemistry and device engineering has driven efficiencies beyond 25% in single-junction architectures (NREL, 2023). This progress can be largely attributed to the unique optoelectronic properties of perovskite materials, such as high absorption coefficients, long carrier diffusion lengths, and defect tolerance (Zhao *et al.,* 2022).

The tandem configuration shown in Figure 2 is especially important because it allows stacking of two absorber materials with complementary bandgaps, effectively capturing a broader spectrum of sunlight and reducing thermalization losses. In this figure, the perovskite top cell absorbs high-energy photons, while the bottom cell, which can be based on silicon, CIGS, or other materials, absorbs lower-energy photons that pass through the perovskite layer. This configuration has been reported to reach efficiencies exceeding 29% under laboratory conditions (Al-Ashouri *et al.,* 2020). Nanostructuring at the perovskite layer and interfaces is critical for achieving such high performance, as it directly influences light harvesting, charge separation, and recombination dynamics.

One of the most important aspects of nanostructured perovskite layers is the control of grain boundaries and crystallinity. Large, well-oriented perovskite grains minimize recombination losses by reducing the density of trap states that can capture charge carriers (Brenner *et al.,* 2020). Various techniques have been developed to achieve such high-quality films, including solvent engineering, additive incorporation, and thermal annealing. For instance, the addition of alkali metal ions or passivating molecules during fabrication can significantly enhance film uniformity and passivate defects, leading to improved stability and higher open-circuit voltages (Turren-Cruz *et al.,* 2018).

Moreover, the interfacial layers between the perovskite and charge transport materials must be carefully designed at the nanoscale to ensure efficient extraction of electrons and holes. Electron transport layers such as TiO_2 nanoparticles, SnO_2 nanocrystals, and fullerene derivatives have been extensively studied for their ability to create favorable band alignment and facilitate charge transfer (Min *et al.,* 2021). Similarly, hole transport layers like Spiro-OMeTAD and doped polymers provide pathways for hole extraction while blocking electrons, further enhancing performance. The figure also implies the need for surface passivation layers, which reduce recombination at interfaces by saturating dangling bonds and mitigating ion migration.

Nanoscale compositional tuning is another crucial strategy demonstrated in this architecture. By partially substituting cations and anions within the perovskite lattice, researchers can adjust the bandgap and stabilize the perovskite phase. For example, the mixed cation perovskite formulation $(FA_{0.85}MA_{0.15})Pb(I_{0.85}Br_{0.15})_3$ has shown enhanced phase stability and improved thermal tolerance compared to methylammonium-only perovskites (Jeong *et al.,* 2021). Incorporating cesium or rubidium cations can further suppress phase segregation and improve long-term operational stability.

While the advances in nanostructuring and compositional engineering have driven rapid improvements in performance, several challenges remain. One of the most significant is the long-term stability of perovskite solar cells under operational conditions. Factors such as moisture, heat, UV light, and ion migration can degrade the perovskite layer and interfacial contacts over time, reducing device efficiency and lifespan (Yuan *et al.,* 2021). Efforts to encapsulate devices with barrier films and introduce robust passivation layers have led to promising improvements, but achieving commercial-grade stability remains an active area of research.

Another key issue is the scalability and reproducibility of nanostructured perovskite films. While spin coating is commonly used in the lab, scalable techniques such as slot-die coating, blade coating, and inkjet printing must be adapted to produce large-area, uniform films with controlled nanostructure (Shao *et al.,* 2022). Additionally, the use of lead-based materials raises environmental and regulatory concerns, motivating the exploration of lead-free alternatives such as tin-based perovskites. However, these alternatives still face significant performance gaps compared to lead-containing perovskites.

Integration with existing silicon photovoltaic manufacturing infrastructure is another critical consideration. Tandem architectures, as depicted in Figure 2, are particularly attractive because they leverage mature silicon technology while adding a high-performance perovskite layer. However, the interconnection of the two cells requires precise control of interface properties, current matching, and thermal management to avoid degradation and losses (Al-Ashouri *et al.,* 2020).

Cost considerations also play an important role in determining the viability of perovskite solar cells for large-scale deployment. While materials costs are relatively low, achieving high yields and uniformity in manufacturing remains challenging. Furthermore, device encapsulation and module integration can add complexity and expense. Developing robust, scalable processing techniques that preserve the unique nanostructured benefits demonstrated in small-scale devices is essential for commercialization. Case studies have highlighted several successful implementations of nanostructured perovskite solar cells. For example, a recent report demonstrated that incorporating passivating agents and tuning the perovskite composition resulted in certified efficiencies over 25% with operational stability exceeding 1,000 hours (Jeong *et al.,* 2021). Other studies have shown that perovskite/silicon tandems can surpass the Shockley–Queisser limit of single-junction silicon cells, offering a pathway to achieving cost-effective, high-efficiency photovoltaics (Min *et al.,* 2021).

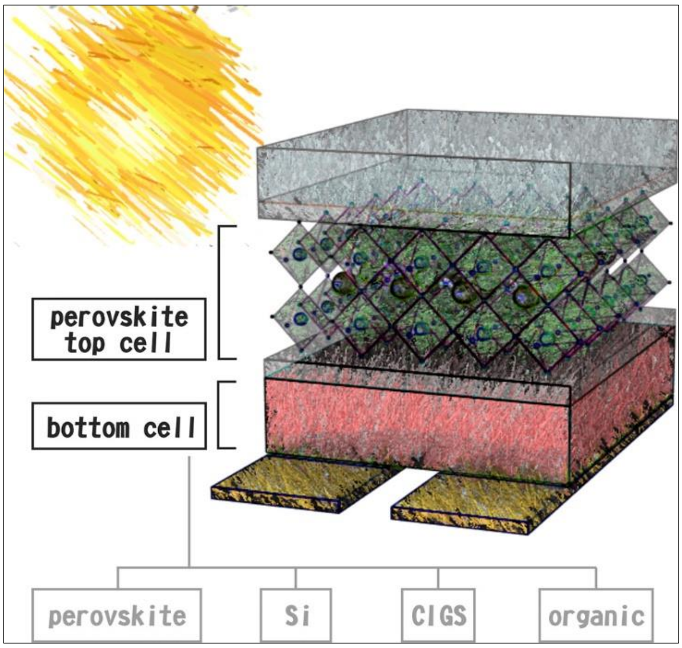

Figure2: Nanostructured Perovskite Architectures Enhancing Light Harvesting in Solar Cells"

This figure depicts nanostructured perovskite layers integrated with electron transport and hole transport materials to improve photovoltaic performance. It highlights grain boundary engineering, surface passivation, and nanoscale compositional tuning that increase efficiency. The schematic shows how reduced recombination and improved charge extraction are achieved through precise nanostructuring. These innovations underpin recent breakthroughs in perovskite solar cell efficiency and scalability.

3.2. Supercapacitors and Batteries (Li-ion, Na-ion, Solid-State)

Electrochemical energy storage technologies are critical in modern applications ranging from portable electronics to electric vehicles and grid-scale storage. Among these, lithium-ion (Li-ion) batteries dominate due to their high energy density, cycle life, and efficiency. Figure 3 illustrates the fundamental working mechanism of a Li-ion battery during charge and discharge cycles.

In a typical Li-ion battery (as shown in Figure 3), the cathode is commonly composed of lithium cobalt oxide ($LiCoO_2$), while the anode is often made of graphite. During the discharge process, lithium ions (Li^+) move from the anode to the cathode through the non-aqueous electrolyte and across the separator, releasing energy. Simultaneously, electrons flow through an external circuit from the anode to the cathode, powering connected devices. During charging, the process is reversed: Li^+ ions are driven back to the anode from the cathode, storing energy chemically for later use (Nitta *et al.,* 2015). The separator, as shown in the figure, plays a crucial role by preventing direct contact between the anode and cathode while allowing ionic flow. The choice of non-aqueous electrolytes enables a wide electrochemical stability window, essential for the high-voltage operation of Li-ion batteries (Xu, 2004).

Beyond Li-ion systems, emerging technologies like sodium-ion (Na-ion) and solid-state batteries are gaining attention. Na-ion batteries, which use sodium instead of lithium, offer cost advantages and abundant raw materials, making them attractive for large-scale storage. However, they typically have lower energy density than Li-ion batteries (Hwang *et al.,* 2017). Solid-state batteries, which use solid electrolytes instead of liquid ones, promise enhanced safety, higher energy density, and thermal stability, but face challenges in interface resistance and manufacturing scalability (Janek & Zeier, 2016). In comparison, supercapacitors store energy through electrostatic processes rather than electrochemical reactions. This results in much faster charge/discharge cycles and higher power density, though at the expense of energy density. While not suitable for long-term energy storage, supercapacitors excel in applications requiring rapid energy delivery or buffering.

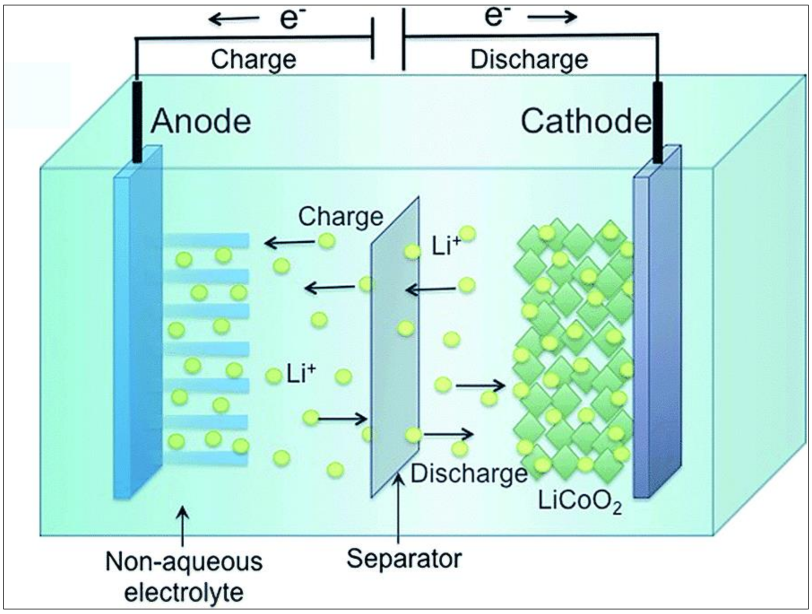

Figure 3: Schematic Illustration of a Lithium-Ion Battery During Charge and Discharge Cycles

This diagram shows the fundamental working principle of a lithium-ion battery. Lithium ions (Li^+) migrate between the anode and cathode through a non-aqueous electrolyte and separator. During discharge, Li^+ moves from anode to cathode, generating electric current. During charging, the ions reverse direction, storing energy within the system.

3.3. Fuel Cells and Hydrogen Production (Photocatalytic/Electrocatalytic Water Splitting)

Fuel cells and hydrogen production technologies are central to the global shift toward sustainable energy. Among the diverse strategies for hydrogen generation, photocatalytic and electrocatalytic water splitting have emerged as highly promising, particularly due to their potential to produce clean hydrogen using solar or electrical energy without harmful emissions. One of the key enablers in enhancing the efficiency of these water-splitting systems is the incorporation of nanostructured materials. By designing catalysts and electrodes at the nanoscale, researchers have been able to unlock performance improvements that are unattainable with bulk materials.

Nanostructuring significantly improves light absorption, surface reactivity, charge transport, and catalytic activity. In photocatalytic systems, nanomaterials such as quantum dots, nanorods, and nanosheets provide increased surface area and reduce the charge diffusion length, leading to more efficient separation and utilization of photogenerated charge carriers. For example, TiO_2 nanorods have demonstrated superior hydrogen evolution performance compared to bulk TiO_2, attributed to better light harvesting and minimized electron-hole recombination (Ma *et al.,* 2014). In electrocatalytic systems, nanostructured materials like transition metal dichalcogenides offer abundant active sites, especially when synthesized as few-layered nanosheets. MoS_2, in particular, exhibits highly active edge sites when reduced to the nanoscale, thereby lowering the overpotential required for hydrogen evolution reactions (Jaramillo *et al.,* 2007).

The benefits of nanostructuring also extend to bandgap engineering and interfacial charge dynamics. By doping or forming heterostructures, researchers can modulate the electronic properties of photocatalysts, thereby enhancing visible light absorption and improving charge separation. These properties are critical in Z-scheme or tandem photocatalytic systems, where multiple semiconductors are coupled to drive both the hydrogen and oxygen evolution reactions efficiently (Hisatomi *et al.,* 2014).

Several case studies underscore the value of nanostructuring in real-world applications. One such example is the $LaFeO_3$–MoS_2 nanocomposite, synthesized via hydrothermal methods, which demonstrates significantly enhanced photocatalytic activity. The heterojunction between $LaFeO_3$ and MoS_2 promotes efficient charge separation and supports Z-scheme water splitting mechanisms, leading to improved hydrogen generation under simulated sunlight (Zhang *et al.,* 2021). Another compelling case is the Fe/MgO–rGO nanohybrid, where iron and magnesium oxides are anchored on reduced graphene oxide sheets. This composite achieves nearly four times the hydrogen production efficiency of traditional TiO_2 under solar irradiation, thanks to the enhanced conductivity and light absorption properties imparted by the rGO (Zhao *et al.,* 2021).

Further supporting the role of nanostructuring, MoS_2 nanosheets combined with graphene have demonstrated impressive electrocatalytic performance, with HER onset potentials as low as 100 mV and Tafel slopes around 40 mV/decade. These improvements are largely attributed to the synergistic interactions between the conductive graphene network and the catalytically active edges of MoS_2 (Voiry *et al.,* 2015). Another noteworthy development is the growth of Ni_3S_2 nanosheets on nickel foam substrates, forming a 3D electrode structure that enables high catalytic activity at low overpotentials, along with excellent mechanical stability and scalability (Wu *et al.,* 2020). Similarly, vertically aligned $W_{0.4}Mo_{0.6}S_2$ on graphene sheets has shown strong durability over 1000 cycles and high hydrogen evolution efficiency, indicating its potential for long-term deployment in electrochemical systems (Voiry *et al.,* 2015).

Despite these promising advances, several challenges hinder the practical deployment of nanostructured systems for large-scale hydrogen production. One of the most persistent issues is stability. Many nanomaterials suffer from photo corrosion, chemical degradation, or detachment from supports under prolonged operation. Semiconductor photocatalysts, for instance, can degrade under continuous UV or visible light exposure. Strategies such as surface passivation, core–shell structures, and protective coatings (e.g., TiO_2 or Al_2O_3 layers) have been developed to mitigate these effects and prolong the lifespan of photocatalysts (Liu *et al.,* 2020; Li *et al.,* 2025).

Cost and scalability also represent major bottlenecks. The synthesis of high-performance nanomaterials often involves expensive precursors or complex fabrication techniques that are not easily scalable. Precious metal-based catalysts like platinum (Pt) and iridium (Ir) remain benchmarks for HER and OER, respectively, but their scarcity and high cost limit commercial viability. To address this, research has shifted toward non-precious alternatives such as transition metal phosphides, nitrides, and sulfides, which offer comparable performance at a fraction of the cost (Morales-Guio & Hu, 2014). Furthermore, scalable synthesis techniques like chemical vapor deposition (CVD), hydrothermal growth, and electrodeposition are being refined to enable large-scale production of nanostructured catalysts and electrodes.

Another major challenge is the integration of nanoscale materials into macroscale devices and systems. Laboratory-scale experiments often involve small electrodes and precise conditions, which may not be easily replicated in industrial settings. Achieving uniform distribution of catalysts over large-area electrodes, maintaining strong adhesion, and ensuring efficient current collection are all critical to real-world application. Innovative approaches, such as using porous foam substrates, 3D printing, and roll-to-roll coating techniques, are being explored to bridge this gap (Jiang *et al.,* 2019). Additionally, photoelectrochemical cells incorporating nanoporous $BiVO_4$ with layered oxygen evolution catalysts have demonstrated successful integration strategies, leading to enhanced water-splitting performance at scale (Kim & Choi, 2014).

In conclusion, nanostructuring has proven to be a transformative approach in the field of photocatalytic and electrocatalytic hydrogen production. By tailoring materials at the nanoscale, researchers have achieved significant gains in catalytic efficiency, light absorption, and system durability. A growing body of case studies confirms the practical benefits of nanostructured composites, including heterojunction engineering, 3D porous frameworks, and conductive supports. Nevertheless, challenges related to long-term stability, production costs, and device integration remain formidable. Addressing these challenges through continued material innovation, scalable manufacturing, and system-level engineering will be essential for realizing the vision of clean, hydrogen-based energy systems on a global scale.

Table 1: "Representative Nanostructured Catalysts for Photocatalytic and Electrocatalytic Hydrogen Production"

System / Catalyst	Nanostructure	Performance Highlights	Key Benefits
$LaFeO_3$–MoS_2	Nanocomposite via hydrothermal synthesis	RhB photodegradation ~96%; improved Z-scheme water splitting	Enhanced charge separation, visible light activity
Fe/MgO–rGO	Fe and MgO nanoparticles on rGO sheets	~4× H_2 generation vs P25 under solar irradiation	Better light absorption and electron transport
MoS_2/RGO	Few-layer MoS_2 nanosheets on graphene	HER onset ~100 mV; Tafel slope ~40 mV/dec	Abundant active sites, high conductivity
Ni_3S_2/Ni foam	3D nanosheet arrays on foam	Overpotentials ~135–255 mV at 10–100 mA/cm²	High stability, large electrochemical surface area
$W_{0.4}Mo_{0.6}S_2$/graphene	Vertically grown TMDs on conductive sheets	HER onset ~96 mV; stable after 1000 cycles	Pt-free, scalable, robust interface design

4. Environmental Remediation

4.1. Photocatalysis for Organic Pollutant Degradation (e.g., dyes, phenols)

Photocatalysis has emerged as a powerful technique for the degradation of persistent organic pollutants such as dyes and phenolic compounds in wastewater. Among various photocatalytic materials, semiconductors like titanium dioxide (TiO_2) and graphitic carbon nitride (g-C_3N_4) have garnered significant attention due to their stability, photocatalytic efficiency, and environmental friendliness. However, the major limitation of TiO_2 is its wide band gap (~3.2 eV), which restricts its activation to the ultraviolet region, comprising only a small fraction of the solar spectrum (Chen *et al.,* 2010). To overcome this, heterojunctions such as TiO_2/g-C_3N_4 have been designed to enhance charge separation, extend light absorption into the visible region, and improve overall photocatalytic performance.

The figure provided shows a schematic diagram of the photocatalytic degradation mechanism of Acid Orange 7 (AO7), a model dye pollutant, using a g-C_3N_4/TiO_2 heterojunction system under visible light irradiation. In this system, both semiconductors absorb visible light and generate photoexcited electron–hole pairs. Due to the suitable band alignment between TiO_2 and g-C_3N_4, electrons from the conduction band (CB) of g-C_3N_4 migrate to the CB of TiO_2, while holes from the valence band (VB) of TiO_2 transfer to the VB of g-C_3N_4. This type II heterojunction (or, in some interpretations, a Z-scheme mechanism) effectively separates photogenerated charge carriers and reduces electron–hole recombination (Zhang *et al.,* 2015).

These separated charge carriers then interact with adsorbed molecules on the catalyst surface. The electrons react with dissolved oxygen (O_2) to form superoxide radicals ($\bullet O_2^-$), while the holes react with water or hydroxide ions (OH^-) to produce hydroxyl radicals (•OH). These reactive oxygen species (ROS) are highly effective in oxidizing and mineralizing organic pollutants into harmless end products such as CO_2 and H_2O (Kamat, 2007). The figure also highlights the redox potentials involved: the CB of g-C_3N_4 is at −1.12 eV, sufficient for O_2 reduction, while the VB of TiO_2 at 2.84 eV supports hydroxyl radical generation. These positions enable efficient ROS formation for pollutant degradation.

Nanostructuring further enhances this process by increasing surface area, providing more active sites for adsorption and reaction, and facilitating carrier mobility. For instance, TiO_2 nanoparticles deposited on g-C_3N_4 nanosheets exhibit improved interfacial contact, which aids in rapid electron transfer and suppresses recombination losses (Dong *et al.,* 2018). Such structural modifications also allow better light harvesting and photon utilization efficiency. A case study by Liang et al. (2018) demonstrated the superior performance of a sulfur-doped TiO_2/g-C_3N_4 composite, which degraded over 95% of methylene blue (MB) dye within 60 minutes under visible light. The enhanced activity was attributed to better light absorption, charge separation, and higher surface area. Furthermore, the catalyst showed excellent stability and reusability over multiple cycles, addressing key practical concerns in photocatalytic applications.

Similarly, phenolic compounds, which are hazardous pollutants in industrial wastewater, can be effectively degraded using TiO_2/g-C_3N_4 photocatalysts. According to a study by Wang *et al.,* (2019), a composite photocatalyst achieved nearly complete degradation of phenol under simulated sunlight in less than 90 minutes. The degradation pathway involved hydroxylation, ring cleavage, and eventual mineralization, as confirmed by intermediates detected via HPLC and LC-MS analysis. While the photocatalytic degradation of organic pollutants using heterojunction photocatalysts like TiO_2/g-C_3N_4 has proven efficient, several challenges remain. One of the primary concerns is photocatalyst regeneration and long-term stability. Photo corrosion, surface fouling by intermediate products, and catalyst deactivation due to agglomeration or phase separation can reduce efficiency over time (Zhou *et al.,* 2020). Moreover, the use of noble metals (e.g., Ag, Pt) to enhance activity raises cost issues and limits scalability.

Environmental and toxicity concerns also need consideration. Though TiO_2 and g-C_3N_4 are generally regarded as safe, certain dopants and by-products from degradation processes may pose toxicity risks if not fully mineralized. Lifecycle assessments are essential to ensure environmental compatibility of the materials and degradation pathways (Nasirian *et al.,* 2021). Scalability and integration with real wastewater treatment systems present additional hurdles. In lab-scale studies, photocatalysis is often tested under ideal conditions with artificial light sources and low pollutant concentrations. Real-world wastewater contains multiple pollutants, variable pH, and suspended solids, which can interfere with photocatalytic activity. To address this, immobilization of photocatalysts on substrates, such as membranes or glass fibers, is being explored to improve practical applicability (Ahmed *et al.,* 2018).

Moreover, green synthesis approaches for these catalysts are gaining attention. Methods such as thermal condensation of urea for g-C_3N_4, hydrothermal growth of TiO_2, and doping via bio-derived agents reduce the environmental footprint of catalyst preparation. These techniques align with principles of sustainable chemistry and enable large-scale production of photocatalysts with minimal environmental impact (Zhou *et al.,* 2020). In conclusion, the use of nanostructured TiO_2/g-C_3N_4 heterojunctions represents a promising approach for the photocatalytic degradation of dyes and phenolic compounds in wastewater. By enhancing charge separation, visible-light absorption, and surface activity, these materials achieve high degradation efficiency and potential for real-world deployment. Continued research into stability, environmental safety, and cost-effective synthesis will be vital to their widespread application in environmental remediation technologies.

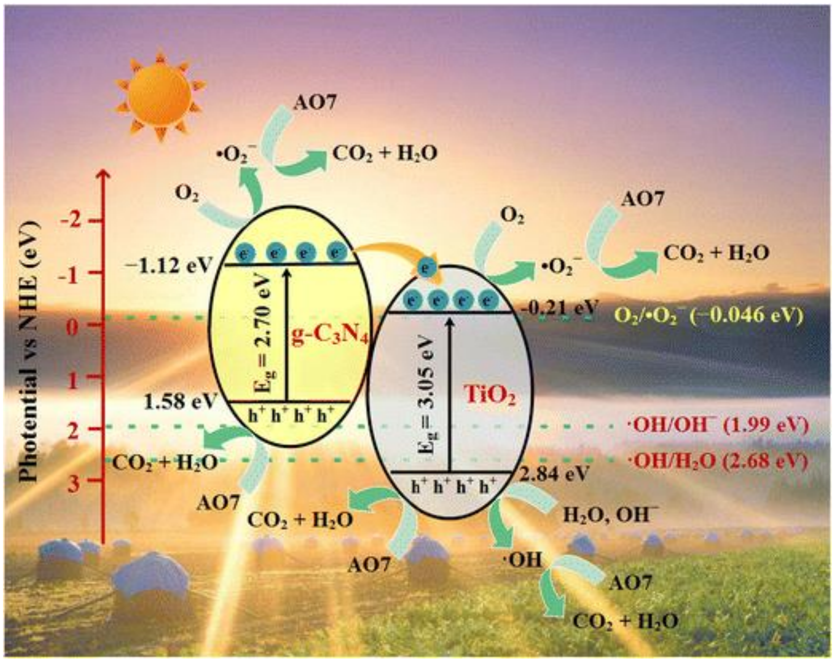

Figure 4: Schematic Diagram of Photocatalytic Degradation of Organic Pollutants via a TiO_2/g-C_3N_4 Heterojunction under Visible Light Irradiation

This figure depicts the mechanism of photocatalytic degradation of organic pollutants, such as dyes or phenolic compounds, using a TiO_2/g-C_3N_4 heterojunction under visible-light irradiation. When illuminated, both semiconductors absorb photons to generate electron-hole pairs; electrons transfer from g-C_3N_4 to TiO_2, while holes move in the opposite direction, forming a type II (or direct S-scheme) junction that enhances charge separation. These separated charges then react with adsorbed pollutant molecules to generate reactive oxygen species (e.g., $\cdot O_2^-$ and $\cdot OH$) that oxidize the pollutants into benign products like CO_2 and H_2O. Nanostructuring increases surface area, improves light absorption, and minimizes charge recombination, significantly boosting photocatalytic efficiency.

4.3 Membrane and Filtration Technologies

Membrane and filtration technologies have become increasingly important for the removal of heavy metals from water, leveraging engineered nanomaterials such as g-C_3N_4, TiO_2, and $ZnFe_2O_4$. A representative figure shows the preparation and application of $ZnFe_2O_4$/g-C_3N_4 heterojunction nanocomposites: $ZnFe_2O_4$ nanoparticles are anchored onto g-C_3N_4 nanosheets via controlled synthesis routes, increasing surface area and functional group density. This configuration enables selective adsorption of heavy metal ions like Pb^{2+} and Cd^{2+} through coordination with –OH and –NH functional groups. Following adsorption, magnetic recovery of $ZnFe_2O_4$ allows for efficient separation of loaded adsorbent using external magnets, enhancing recyclability and simplifying regeneration.

Nanomaterials like $ZnFe_2O_4$ and g-C_3N_4 enhance adsorption via synergistic effects. $ZnFe_2O_4$ offers magnetic response facilitating recovery and high surface area, while g-C_3N_4 contributes functional sites and hydrophilicity (Subramaniam, 2019). Studies have shown tunable adsorption capacities; for instance, Mg-doped $ZnFe_2O_4$ nanoparticles prepared via sol–gel methods recorded capacities up to 143 mg/g for Pb^{2+}, 117 mg/g for Cu^{2+}, and 77 mg/g for Cd^{2+} (Jethave *et al.,* 2019). Adsorption kinetics followed pseudo-second order models, indicating chemisorption as the dominant mechanism.

g-C_3N_4-based membranes have been shown to achieve >98% rejection rates for heavy metal ions, even at high concentrations such as 2500 mg/L Cu^{2+}. The mechanism comprises a combination of adsorption by amino functional groups, electrostatic repulsion, and steric hindrance. Under light exposure, the g-C_3N_4 membrane also promotes photocatalytic reduction of metal ions, converting them to elemental form and thereby intensifying removal efficiency (Zhao *et al.,* 2022). This dual adsorption-photoreduction-filtration mechanism greatly enhances long-term performance and reduces secondary pollution risk.

The synthesis of these nanomaterials frequently employs eco-friendly routes. For $ZnFe_2O_4$, green precursors derived from plant extracts such as lemon juice, Aegle marmelos, or Lawsonia inermis have been used to avoid toxic solvents and harsh reagents, contributing to sustainable nanomaterial fabrication (Subramaniam, 2019; Pagar *et al.,* 2023). Similarly, g-C_3N_4 is commonly produced via thermal polycondensation of urea or melamine, offering a low-cost, green synthesis pathway. Integration with support matrix or biomass-derived materials decreases carbon footprint and encourages scalable production. Regeneration and reusability are crucial for practical application. The magnetic nature of $ZnFe_2O_4$ allows for rapid separation of adsorbent post-treatment. Regeneration can be achieved via simple acid or base washing, restoring adsorption sites for repeated cycles. Most studies report sustained removal efficiency (80–90%) after five regeneration cycles, with minimal loss in capacity. However, repeated cycles can lead to gradual structural degradation or surface fouling, emphasizing the need for robust functionalization and protective coatings.

Toxicity considerations are also important. While $ZnFe_2O_4$ is often described as biocompatible at low concentrations, the release of Zn or Fe ions and any residual synthesis byproducts must be monitored. Similarly, carbon nitride-based membranes should be evaluated for leaching of nitrogen-containing compounds or incomplete pollutants. Life cycle analyses and ecotoxicological assessment are essential to validate environmental safety and compliance with regulatory standards. Scalability remains a major challenge. Many reported studies utilize batch systems at laboratory scale with ideal water matrices. In real wastewater, competing ions, high salinity, pH variation, and suspended solids can reduce adsorption performance. Membrane fouling due to organic or microbial matter may block pores or shield active sites, decreasing permeability and requiring frequent cleaning. Strategies like immobilizing nanomaterial onto support fibers, implementing anti-fouling coatings, or using periodic back-flush protocols are being explored to address these issues (Subramaniam, 2019; Zhao *et al.,* 2022).

Compared to conventional adsorbents such as activated carbon or ion-exchange resins, nanomaterial-based membranes and magnetic adsorbents offer faster kinetics, higher specific capacities, and easier post-treatment separation. For instance, $ZnFe_2O_4$/rGO or $ZnFe_2O_4$@g-C_3N_4 composites show adsorption kinetics twice as fast, with comparable or greater capacity. The combination of adsorption, filtration, and when applicable, photocatalytic reduction, constitutes a multifunctional approach that is well-suited to modern water treatment requirements. Cost analysis indicates that while nanosynthesis may increase material costs compared to conventional adsorbents, the advantages of regeneration and reduced sludge generation can offset expenses. Moreover, green synthesis and abundant precursors like plant extracts, urea, or iron/zinc salts reduce upstream costs. Pilot-scale demonstrations of $ZnFe_2O_4$-based adsorbents and g-C_3N_4 membranes are emerging, showing promise for industrial adaptation.

In summary, membrane and filtration technologies incorporating nanomaterials such as $ZnFe_2O_4$ and g-C_3N_4 provide a compelling strategy for removing heavy metal ions from water. They deliver high adsorption capacities, magnetic recoverability, and multifunctional mechanisms (adsorption plus photocatalytic action), while green synthesis routes support environmental and economic sustainability. Nonetheless, challenges such as regeneration durability, toxicity risk, fouling, and scale-up remain. Continued work on material stabilization, anti-fouling integration, life-cycle assessment, and real wastewater testing will be vital in translating laboratory successes into large-scale environmental remediation solutions.

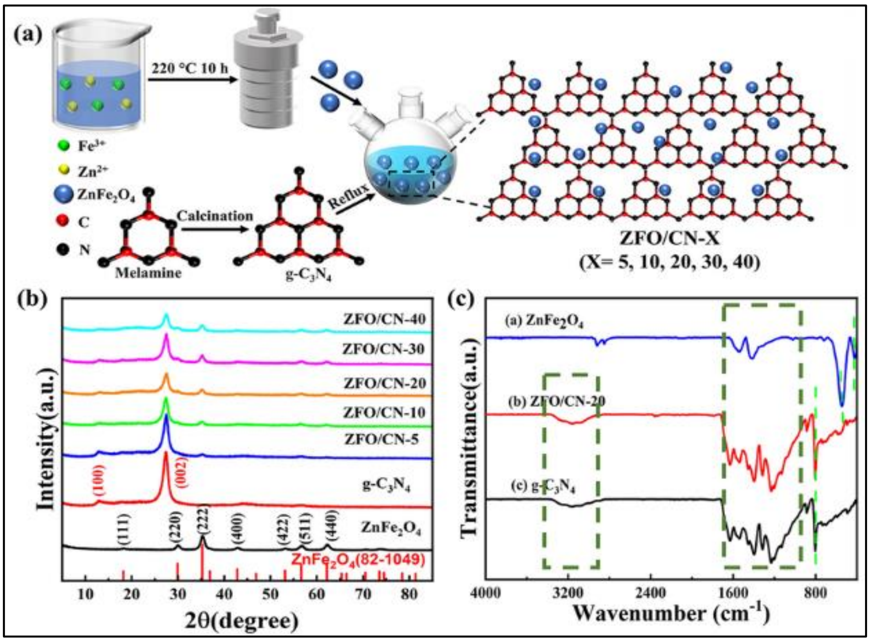

Figure 5: Nanomaterial-Based Adsorption Mechanisms for Heavy Metal Removal Using Magnetic Nanoferrite Adsorbents

This schematic demonstrates how magnetic ferrite nanoadsorbents (e.g., $ZnFe_2O_4$, Ni–Zn ferrites) selectively bind heavy metal ions such as Pb^{2+} and Cd^{2+} from contaminated water. Surface functional groups (e.g., –OH, $–NH_2$) form coordination or ion-exchange bonds with metal ions, enabling efficient removal. Following adsorption, magnetic properties allow rapid separation of the loaded adsorbent using an external magnet. The figure also highlights adsorption capacities and recyclability, underscoring eco-friendly synthesis and regeneration potential.

Catalysis and Green Chemistry

Heterogeneous Catalysis in Organic Reactions

Heterogeneous catalysis plays a foundational role in both traditional chemical manufacturing and modern green chemistry practices. In heterogeneous systems, the catalyst exists in a different phase than the reactants—commonly a solid catalyst interacting with liquid or gaseous substrates. This phase separation allows for easy separation and reuse of the catalyst, often without significant loss of activity, making the system more environmentally and economically viable. The solid catalyst's robustness also permits its application under continuous flow conditions, a key feature for scalable green industrial processes.

One of the most impactful uses of heterogeneous catalysis in organic chemistry lies in carbon–carbon (C–C) and carbon–heteroatom (C–X) bond-forming reactions, which are the backbone of constructing complex molecular architectures in pharmaceuticals, agrochemicals, and fine chemicals. Common examples include the Suzuki–Miyaura, Heck, and Sonogashira couplings, traditionally conducted with homogeneous palladium complexes. These reactions have been successfully adapted for heterogeneous systems using supported catalysts such as palladium on carbon (Pd/C), metal oxides, and metal nanoparticles embedded in solid matrices. For example, Pd/C has proven effective in aqueous media, a significant improvement over traditional systems that require toxic organic solvents. The replacement of phosphine ligands with solid supports like activated carbon, alumina, zeolites, or metal-organic frameworks (MOFs) further contributes to reducing the environmental impact of these reactions (Balanta *et al.,* 2011; Dhakshinamoorthy *et al.,* 2012).

Table 1 illustrates several representative heterogeneous catalysts used in C–C coupling reactions and their relevant green chemistry parameters such as solvent usage, temperature, recyclability, and associated references.

Table 2: Representative Heterogeneous Catalysts in C–C Coupling Reactions

Catalyst Type	Reaction	Solvent	Temp (°C)	Recyclability	Reference
Pd/C	Suzuki–Miyaura	Water/Ethanol	80	High	Balanta *et al.,* 2011
Pd@MOF	Heck	Ionic liquids	120	Moderate	Dhakshinamoorthy *et al.,* 2012
Ni/Graphene	Kumada–Corriu	THF	60	High	Liu *et al.,* 2018
Au/TiO_2	Oxidation of Alcohols	Water	90	High	Corma & Garcia, 2008
Cu/Al_2O_3	Ullmann Coupling	DMSO	100	Moderate	Ley & Thomas, 2003

Beyond coupling reactions, heterogeneous catalysts have proven valuable in hydrogenation, oxidation, and esterification processes. For example, platinum and nickel-based catalysts are routinely used for the hydrogenation of alkenes and carbonyl compounds. These reactions are integral to producing fragrances, pharmaceuticals, and intermediates for polymers. A key advancement has been the development of supported noble metal catalysts capable of operating under aqueous or solvent-free conditions, significantly reducing environmental hazards and process costs.

Environmental advantages of heterogeneous catalysis in green chemistry are manifold. First, the catalyst can often be reused multiple times without significant loss in performance. This reusability not only conserves raw materials but also diminishes the generation of hazardous waste. Second, these systems typically exhibit high selectivity, which minimizes the formation of by-products and reduces the need for extensive downstream purification. Third, the ability to conduct reactions under mild conditions—lower temperatures and pressures—translates to energy savings and improved safety profiles. Additionally, the immobilization of catalysts on solid supports enhances their stability, prevents metal leaching into products, and facilitates integration into continuous-flow reactors (Beale *et al.,* 2010).

Despite these advantages, there are challenges associated with heterogeneous catalysis that must be addressed for its widespread adoption in green chemical manufacturing. One primary concern is catalyst deactivation through fouling, sintering, or poisoning, which can reduce efficiency and require energy-intensive regeneration processes. Another challenge is achieving uniform active site distribution and optimal surface area on the catalyst, which are critical factors for activity and selectivity. Furthermore, characterizing and understanding the structure–activity relationships of solid catalysts remains a complex endeavor due to the inherent heterogeneity of their surfaces. Tools such as operando spectroscopy, in situ X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), and synchrotron radiation-based methods have become essential in elucidating catalytic mechanisms and active site dynamics (Beale *et al.,* 2010).

Selectivity remains a persistent research gap, especially in multifunctional organic molecules where site-selective activation is critical. For example, hydrogenation of α, β-unsaturated carbonyl compounds often requires selective reduction of the C=C bond without affecting the carbonyl group—a challenge for non-tuned heterogeneous systems. Researchers are working on designing bifunctional catalysts and catalysts with well-defined metal-support interactions to address this issue.

Another vital area of research is the recyclability and long-term stability of heterogeneous catalysts. Although many systems demonstrate recyclability in initial cycles, performance often drops due to metal leaching, aggregation, or surface fouling. The development of highly robust supports such as covalent organic frameworks (COFs), mesoporous silicas, and magnetic nanoparticles has shown promise in extending catalyst life cycles. Furthermore, engineering catalysts compatible with reactor systems such as fixed-bed and microchannel reactors is crucial for translating laboratory findings into scalable, sustainable processes (Zhou *et al.,* 2017).

The integration of heterogeneous catalysis with renewable feedstocks and green energy sources is also emerging as a critical area. For instance, coupling catalytic biomass conversion with solid acid/base catalysts offers a route to produce platform chemicals like furfural, levulinic acid, and 5-hydroxymethylfurfural (HMF) from lignocellulosic biomass. Solid catalysts like sulfonated carbons or modified zeolites are being developed to tolerate impurities inherent in biomass and to operate in aqueous environments, further enhancing their environmental compatibility (Melero *et al.,* 2009).

In summary, heterogeneous catalysis offers significant advantages for advancing the principles of green chemistry through improved efficiency, selectivity, and reusability, while reducing hazardous waste and energy consumption. However, for broader adoption and impact, continued research is required to overcome current limitations related to catalyst stability, mechanistic understanding, and system integration. Innovations in catalyst design, characterization, and process intensification hold the key to unlocking the full potential of heterogeneous systems for sustainable chemical production.

4.2. Electrocatalysis and Photocatalysis

Electrocatalysis and photocatalysis have emerged as critical technologies for implementing green chemistry principles in chemical synthesis, energy conversion, and environmental remediation. Unlike traditional thermally driven processes, these catalytic strategies utilize renewable electricity or solar energy to drive chemical transformations under milder, safer, and more sustainable conditions. Their rapid development over the past decade has been motivated by global efforts to decarbonize the chemical industry, utilize CO_2 as a feedstock, and shift towards electrified or solar-driven manufacturing platforms.

Electrocatalysis accelerates redox reactions at the interface of electrodes and electrolytes using applied potentials. This approach has enabled scalable production of key molecules such as hydrogen, oxygen, ammonia, and carbon-based fuels or intermediates from water, nitrogen, and carbon dioxide, respectively. A notable example is water electrolysis, where the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are catalyzed by solid-state materials like NiFe hydroxides, transition metal phosphides, or doped carbons. In recent years, researchers have developed low-cost, highly active non-precious electrocatalysts that rival or surpass traditional noble metals like Pt and Ir (Zhao *et al.,* 2022). For example, transition metal–nitrogen–carbon (M–N–C) single-atom catalysts have shown remarkable performance for OER and CO_2 electroreduction due to their high density of active sites and tunable coordination environments (Xie *et al.,* 2020).

Electrocatalysis also offers a direct route to decarbonization when coupled with renewable electricity. For instance, electrochemical CO_2 reduction (CO_2RR) transforms waste CO_2 into value-added chemicals such as carbon monoxide, methane, ethylene, ethanol, and formic acid. This process provides an avenue for carbon capture and utilization (CCU) in a closed-loop, net-zero carbon cycle (Garza *et al.,* 2019). Copper-based catalysts remain the most promising for forming multicarbon products like ethylene and propanol, while silver and tin-based systems show high selectivity toward CO and formate, respectively. However, challenges persist in tuning product selectivity, reducing overpotentials, and improving catalyst stability in long-term operation. Recent advances have included interface engineering, nanoarchitecturing, and defect regulation to direct electron pathways and modulate local pH near the catalyst surface (Zhang *et al.,* 2023).

On the other hand, photocatalysis leverages light energy—typically sunlight or artificial visible light—to activate semiconductors that mediate chemical transformations. Upon illumination, photoactive materials like TiO_2, graphitic carbon nitride (g-C_3N_4), $BiVO_4$, and metal–organic frameworks (MOFs) generate electron-hole pairs that drive oxidation or reduction reactions on their surfaces. Photocatalysis is widely used in pollutant degradation, water splitting, and increasingly in synthetic organic chemistry, offering metal-free and mild reaction conditions (Kumar *et al.,* 2021).

The use of sunlight as a sustainable energy source makes photocatalysis particularly attractive for decentralized or off-grid applications. For example, g-C_3N_4-based photocatalysts have demonstrated visible-light-driven hydrogen generation from water and photocatalytic oxidation of alcohols to aldehydes or ketones under ambient conditions. Meanwhile, Bi-based materials and doped perovskites are gaining attention for visible-light photocatalytic CO_2 reduction and nitrogen fixation (Li *et al.,* 2021). The application of photocatalysis in pharmaceutical degradation and wastewater treatment also aligns with circular economy goals, as it enables the breakdown of persistent contaminants without secondary pollution.

Hybrid photoelectrocatalytic systems—integrating photocatalysis and electrocatalysis—are also being actively developed to improve reaction rates, selectivity, and energy efficiency. In photoelectrochemical (PEC) water splitting, semiconductor photoanodes (e.g., $BiVO_4$, WO_3) harvest sunlight to drive OER, while HER occurs at dark cathodes like Ni–Mo alloys under applied bias. These systems offer an elegant way to directly store solar energy in the form of hydrogen, with several lab-scale demonstrations showing over 10% solar-to-hydrogen (STH) efficiency under simulated sunlight (Fang *et al.,* 2023).

Nevertheless, both electrocatalysis and photocatalysis still face significant challenges. Electrocatalysts often suffer from limited selectivity and catalyst degradation, particularly in complex multi-electron reactions such as CO_2RR and nitrogen reduction (NRR). Identifying active sites, understanding reaction pathways, and suppressing competitive reactions like HER remain ongoing research priorities. Operando characterization techniques and density functional theory (DFT) simulations have helped reveal that catalyst surfaces undergo dynamic changes during operation, impacting performance and stability (Qiao *et al.,* 2020).

In photocatalysis, rapid charge carrier recombination, poor light absorption in the visible range, and catalyst photocorrosion are limiting factors. Strategies such as heterojunction engineering, co-catalyst loading, and plasmonic enhancement using noble metals (e.g., Ag, Au) have been explored to boost quantum efficiency and expand light utilization. However, achieving long-term photostability and high turnover numbers under real solar conditions remains a challenge for commercialization (Li *et al.,* 2023).

The table below summarizes recent representative catalysts used in green electrocatalytic and photocatalytic applications, including their compositions, targeted reactions, advantages, and corresponding references from 2017–2025.

The evolution of electrocatalysis and photocatalysis continues to be shaped by cross-disciplinary innovations. Machine learning and AI-based screening of catalysts, coupled with robotic synthesis and high-throughput electrochemical testing, are beginning to accelerate discovery cycles. Moreover, coupling catalytic systems with microreactors, membrane separators, and solar concentrators is improving scalability and process integration. Research is also expanding into tandem systems that integrate CO_2 capture and conversion in one step, or dual-functional electrodes that perform oxidation and reduction simultaneously in divided cells.

Table 3: Recent Electrocatalysts and Photocatalysts in Green Chemistry Applications

Catalyst Type	Composition	Target Reaction	Energy Source	Key Benefits
NiFe LDH	Ni–Fe hydroxide	Oxygen Evolution (OER)	Electricity	High activity, earth-abundant, scalable
Cu–Ag Bimetallic	Cu–Ag alloy nanoparticles	CO_2 Reduction to Ethylene	Electricity	Enhanced selectivity, low overpotential
Fe–N–C Single Atom	Fe in N-doped carbon matrix	Oxygen Reduction (ORR)	Electricity	Pt-free, tunable coordination, high durability
g-C_3N_4 Doped with K	K-doped carbon nitride	Photocatalytic H_2 production	Visible Light	Metal-free, stable under solar irradiation
$BiVO_4$/NiOOH Hybrid	$BiVO_4$ photoanode + NiOOH	PEC Water Splitting	Solar + Bias	Efficient solar H_2 generation
Ti_3C_2–MOF Composite	2D MXene + MOF	Photocatalytic Organic Oxidation	Visible Light	High surface area, enhanced charge separation
Co–Ni Phosphide	CoNiP nanoparticles	HER in acidic media	Electricity	Stable, low-cost, acid-resistant

4.3. Enzyme-Mimicking Nanozymes

Nanozymes—nanomaterials with enzyme-like catalytic properties—have rapidly emerged as a promising frontier in green chemistry and catalysis. These materials bridge the gap between biological and synthetic catalysts by offering the specificity and efficiency of enzymes with the robustness and scalability of traditional heterogeneous catalysts. Since their discovery in the early 2000s, the field of nanozymes has evolved dramatically, particularly since 2017, driven by innovations in material science, nanotechnology, and sustainable chemistry. Enzyme-mimicking nanozymes present unique opportunities for developing environmentally benign and cost-effective catalytic systems that can be employed in a range of applications including chemical synthesis, environmental remediation, biosensing, and even artificial photosynthesis.

Nanozymes typically exhibit catalytic behaviors that mimic natural oxidoreductases (e.g., peroxidase, oxidase, catalase), hydrolases, and more recently, even multienzyme cascade reactions. Among these, peroxidase-like nanozymes have received the most attention due to their potential in mimicking key oxidative processes used in both biosystems and synthetic chemistry. These artificial enzymes often use transition metal oxides (e.g., Fe_3O_4, CeO_2, MnO_2), noble metals (e.g., Au, Pt), carbon-based nanomaterials (e.g., graphene oxide, carbon dots), and MOFs or composites as the active matrix for catalysis (Zhang *et al.,* 2021).

Compared with traditional catalysts—including both homogeneous catalysts like organometallic complexes and heterogeneous catalysts like supported metals—nanozymes offer several advantages. First, they demonstrate enzyme-like activity under mild conditions such as physiological pH and ambient temperature, aligning with the green chemistry goal of minimizing energy input. Second, they are typically more stable than natural enzymes, which are prone to denaturation under harsh conditions. Nanozymes can function in a wide range of pH, temperatures, and solvent systems, making them ideal for applications in complex and industrial environments. Third, unlike homogeneous catalysts, nanozymes are easily recoverable and recyclable due to their particulate or solid form. Additionally, nanozymes are often more cost-effective and less toxic than traditional catalysts, especially those involving rare or heavy metals (Gao *et al.,* 2019).

Mechanistically, the enzyme-like activity of nanozymes arises from surface-confined redox centers, defect sites, and electronic structure modulation at the nanoscale. Unlike natural enzymes, which rely on highly evolved protein structures and active sites with defined geometries, nanozymes function through surface-dominated electron and proton transfer mechanisms. For example, Fe_3O_4 nanoparticles exhibit peroxidase-like activity by catalyzing the conversion of H_2O_2 into hydroxyl radicals (•OH), analogous to the activity of horseradish peroxidase (HRP). Similarly, cerium oxide nanozymes switch between Ce^{3+} and Ce^{4+} oxidation states to mimic catalase and superoxide dismutase (SOD) activity. Recent studies have shown that doping, morphology control, and heterostructure formation can fine-tune catalytic activity by modifying the electronic environment around the active sites (Huang *et al.,* 2023).

One of the most exciting developments is the creation of multifunctional nanozymes capable of catalyzing multi-step or cascade reactions. For instance, MOF-derived nanozymes have been engineered to mimic oxidase and peroxidase in tandem, enabling one-pot oxidation of glucose to gluconic acid and subsequent detection via colorimetric assays. These systems have potential applications not only in biosensing but also in green organic synthesis, where cascade catalysis can eliminate intermediate separation steps, thus enhancing atom economy and reducing waste (Li *et al.,* 2022).

Despite these advances, several key research gaps hinder the broader adoption of nanozymes in industrial green chemistry. One persistent limitation is selectivity. While natural enzymes are highly specific due to their well-defined active sites and substrate channels, nanozymes typically exhibit broad substrate scopes, which can be a disadvantage in complex synthetic or biological systems where specificity is critical. Enhancing substrate recognition through surface functionalization or biomimetic structural engineering is a current focus in the field (Wei *et al.,* 2021).

Another challenge is recyclability and long-term stability. While nanozymes are generally more robust than protein-based enzymes, they can still undergo surface passivation, aggregation, or leaching in repeated cycles. This is particularly problematic in liquid-phase catalysis or when dealing with reactive intermediates. To address this, researchers are developing encapsulation strategies using porous supports, polymer shells, or covalent organic frameworks (COFs) to protect the nanozymes while maintaining access to reactants. For instance, Fe_3O_4@MOF hybrid nanozymes have shown up to 10 catalytic cycles with minimal activity loss in oxidative organic reactions (Sun *et al.,* 2023).

Integration of nanozymes with reactor systems and flow chemistry platforms remains an underexplored area. Most studies to date are conducted in batch systems or model aqueous media. However, for nanozymes to be viable in industrial-scale green chemistry applications, they must be compatible with continuous flow reactors, membrane reactors, and electrochemical systems. Immobilization on reactor surfaces or within porous monoliths is one approach to enabling such integration, but optimizing mass transport and catalytic efficiency remains a bottleneck (Wang *et al.,* 2024).

Another emerging opportunity is in photo- and electro-nanozymes—nanozymes that combine light or electricity-driven catalysis with enzyme-mimicking functionality. These systems could bridge the fields of photocatalysis, electrocatalysis, and enzymology by enabling spatiotemporally controlled catalysis. For example, gold-based nanozymes that mimic peroxidase activity can be photoactivated to initiate substrate oxidation with higher spatial resolution, which is useful in both synthetic chemistry and therapeutic applications (Tang *et al.,* 2020).

The table below summarizes representative enzyme-mimicking nanozymes developed since 2017, their catalytic targets, advantages, and corresponding references.

Table 4: Recent Enzyme-Mimicking Nanozymes and Their Catalytic Properties

Nanozyme Type	**Composition**	**Mimicked Enzyme**	**Application Area**	**Key Advantages**
Iron Oxide (Fe_3O_4)	Fe_3O_4 nanoparticles	Peroxidase	Oxidative catalysis, sensing	Magnetic recovery, broad substrate scope
Cerium Oxide	CeO_2 nanoparticles	Catalase, SOD	ROS scavenging, biosensing	Redox cycling (Ce^{3+}/Ce^{4+}), stability
MOF-derived	Fe@MOF	Peroxidase cascade	One-pot green oxidation	Porous, tunable, multi-enzyme mimicry
Carbon Dots	N-doped carbon nanodots	Oxidase	Alcohol oxidation, bioimaging	Metal-free, visible light responsive
Pt–Pd Alloy Nanozymes	PtPd bimetallic nanoparticles	Multienzyme mimicry	Organic synthesis, degradation	High activity, electron transfer efficiency
Au Nanocluster	Au clusters on MOFs	Peroxidase	Photo-responsive catalysis	Light-activated, recyclable
Fe_3O_4@COF Composite	Fe_3O_4 core, COF shell	Peroxidase	Flow reactor compatibility	Enhanced stability, reactor integration

In conclusion, enzyme-mimicking nanozymes represent a transformative platform for green chemistry, offering the potential for selective, low-energy, and recyclable catalytic systems. Their ability to function under ambient conditions, combined with tunable nanostructures and functional interfaces, positions them as next-generation catalysts for sustainable synthesis and environmental remediation. However, key limitations such as substrate selectivity, long-term recyclability, and integration into continuous processes need to be addressed through interdisciplinary research at the interface of catalysis, nanomaterials, and reactor engineering. With continued progress, nanozymes may not only complement but, in specific scenarios, outperform traditional enzyme and metal catalyst systems in green chemistry.

5. Biomedical and Pharmaceutical Applications

5.1. Targeted Drug Delivery and Controlled Release

Targeted drug delivery using stimuli-responsive nanoparticles has become one of the most transformative strategies in pharmaceutical science and nanomedicine. These systems are designed to enhance the localization, retention, and controlled release of therapeutic agents specifically at disease sites, reducing off-target toxicity and improving treatment efficacy. Stimuli-responsive nanocarriers are engineered to remain inert under physiological conditions and become activated only in response to specific biological or external triggers, such as pH, redox environment, enzyme concentration, temperature, light, ultrasound, or magnetic fields.

Figure 6 clearly illustrates the design and functional mechanism of stimuli-responsive nanoparticles for biomedical applications. It shows how nanocarriers are engineered to respond to both endogenous stimuli (e.g., pH, redox potential, enzymes) and exogenous stimuli (e.g., light, temperature, ultrasound, magnetic field). The nanoparticles are functionalized to deliver therapeutic agents with high precision and are utilized in applications such as bio-imaging, therapy, and general biomedicine. Different nanostructures, including dendrimers, polymeric nanoparticles, gold nanoparticles, iron oxide nanoparticles, and quantum dots, are used as platforms depending on the required function and environment.

Over the last decade, the use of nanotechnology in drug delivery has addressed several fundamental challenges in pharmacotherapy, including poor bioavailability, non-specific distribution, and premature drug degradation. In particular, tumor microenvironments provide ideal conditions for the activation of such nanosystems. The acidic pH (~6.5–6.8), overexpressed enzymes (e.g., MMPs, cathepsins), and high glutathione concentration in tumor cells relative to healthy cells offer endogenous cues that can trigger drug release from engineered nanoparticles (Li *et al.,* 2019). These triggers can be exploited for intracellular release, enhancing the cytotoxic effect at the site of action while minimizing systemic toxicity.

Passive targeting through the enhanced permeability and retention (EPR) effect remains one of the foundational principles of nanomedicine. Tumor tissues and inflamed sites often have leaky vasculature and impaired lymphatic drainage, enabling nanoparticles within the size range of 10–200 nm to accumulate selectively in these regions (Yang *et al.,* 2020). While EPR improves accumulation, active targeting is often incorporated to enhance specificity. This is achieved by functionalizing the surface of nanoparticles with ligands such as antibodies, peptides, folic acid, transferrin, or aptamers that recognize overexpressed receptors on the target cells (Chen *et al.,* 2021).

Upon successful accumulation at the diseased site, the key challenge becomes controlling the release of the therapeutic agent. pH-responsive nanoparticles utilize acid-labile bonds such as hydrazone, imine, or acetal linkers that break down in acidic microenvironments to release their cargo (Zhang *et al.,* 2022). Similarly, redox-responsive carriers incorporate disulfide bonds or thiol-sensitive moieties that degrade in high-glutathione environments, commonly found in tumor cells, leading to rapid intracellular drug discharge (Liu *et al.,* 2018). Enzyme-responsive systems use peptide or polysaccharide linkers that are selectively degraded by overexpressed enzymes at the disease site, enabling site-specific release with high selectivity (Wang *et al.,* 2019).

Exogenous stimuli such as near-infrared (NIR) light, magnetic fields, ultrasound, or temperature changes provide external control over drug release, allowing real-time spatiotemporal regulation. Light-responsive nanoparticles often incorporate gold nanoshells or carbon-based materials that convert light energy into heat, triggering structural transformations or bond cleavage (Mi, 2020). Magnetic nanoparticles, typically iron oxide-based, can be heated by alternating magnetic fields to enable thermo-responsive release or even induce hyperthermia in tumor tissues (Gupta *et al.,* 2019). Ultrasound-mediated release involves cavitation and mechanical stress that disrupt the nanocarrier structure, facilitating drug release from liposomes, micelles, or nanogels (Tang *et al.,* 2021).

A new trend in drug delivery involves dual or multi-stimuli-responsive systems. For example, nanoparticles that are both pH- and temperature-sensitive offer greater control and more refined targeting. These systems are particularly effective for tumors that exhibit both abnormal pH and higher local temperatures due to increased metabolism. Incorporating multiple triggers also ensures a higher level of specificity and minimizes premature drug leakage in normal tissues (Kumar *et al.,* 2022). Different nanoparticle platforms are used based on their intended application. Polymeric nanoparticles, such as those made from PLGA, PEG, or chitosan, are biodegradable and biocompatible, making them suitable for systemic administration. Dendrimers, with their highly branched architecture, provide excellent surface functionality and are ideal for multivalent ligand attachment. Metallic nanoparticles like gold (AuNPs) and iron oxide (Fe_3O_4) offer unique optical and magnetic properties, enabling simultaneous therapy and imaging (theranostics). Quantum dots are often employed for bioimaging due to their tunable fluorescence and photostability, though their toxicity remains a concern in clinical applications.

Figure 6 integrates all of these concepts into one concise schematic. It begins by dividing stimuli into endogenous and exogenous categories, then illustrates their interaction with nanoparticle platforms to produce a stimuli-responsive nanocarrier. From there, the figure maps the pathway of therapeutic deployment toward three major biomedical applications: bio-imaging, therapy, and general drug delivery. It also categorizes nanoparticles into types—gold, iron oxide, quantum dots, dendrimers, and polymers—highlighting the versatility of nanotechnology in medicine.

Recent studies have validated the efficacy of such systems in preclinical models. For instance, lectin-conjugated mesoporous silica nanoparticles with pH-sensitive acetal gates achieved higher tumor selectivity and drug retention compared to non-targeted carriers in osteosarcoma models (Martinez-Carmona *et al.,* 2021). Similarly, PEGylated liposomes incorporating disulfide linkers for redox sensitivity showed superior tumor penetration and lower systemic toxicity in breast cancer models (Lee *et al.,* 2018). In another example, thermosensitive liposomes activated by mild hyperthermia released doxorubicin precisely at tumor sites and significantly improved survival in mouse models (Tang *et al.,* 2021).

However, the translation of these smart systems into clinical settings faces considerable challenges. One major limitation is rapid clearance by the mononuclear phagocyte system (MPS), primarily in the liver and spleen. This reduces systemic circulation time and limits bioavailability at the disease site. Surface modification with PEG or zwitterionic polymers has been widely used to evade immune recognition, although anti-PEG immune responses are increasingly being reported (Zhou *et al.,* 2020). Additionally, the long-term toxicity, biodistribution, and degradation pathways of many synthetic nanoparticles are still not fully understood. Reproducibility and scalability of synthesis are also critical barriers. Uniformity in size, surface charge, and ligand density is essential for consistent pharmacokinetics and therapeutic outcomes. Regulatory frameworks are yet to catch up with the complexity of multifunctional nanoplatforms, and approval processes remain lengthy and uncertain. Moreover, while in vitro and animal studies often show promising results, human physiology is far more complex, and nanoparticle behavior can differ significantly in clinical trials.

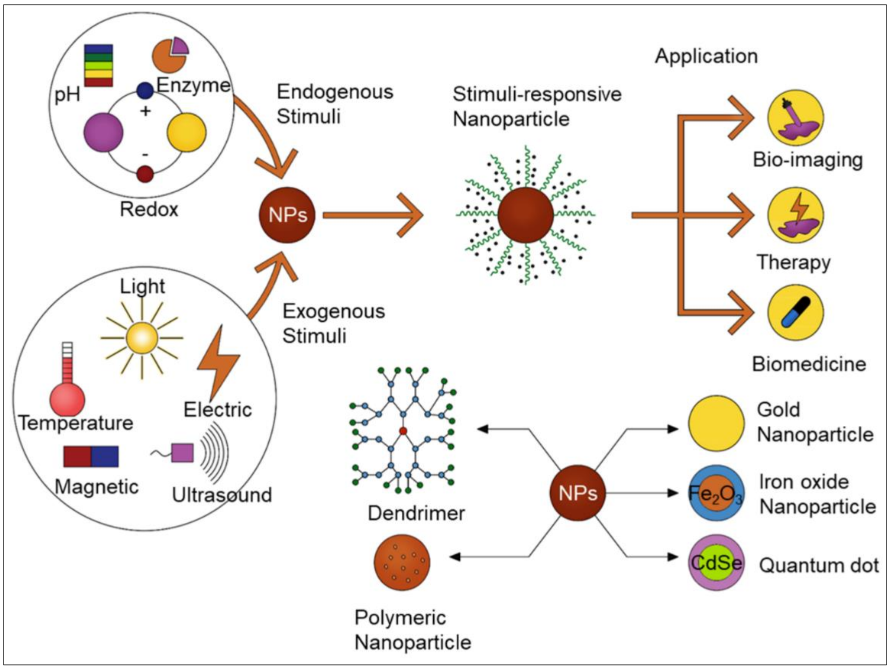

Figure 6: Schematic of Nanoparticle-Mediated Targeted Drug Delivery and Stimuli-Responsive Release

This schematic illustrates functionalized nanoparticles that accumulate at target tissues via the enhanced permeability and retention (EPR) effect and ligand–receptor interaction, ensuring minimized systemic exposure. It depicts multiple stimuli-responsive release mechanisms—pH-triggered bond cleavage, enzyme-mediated degradation, and temperature-sensitive carrier destabilization—to facilitate precise intracellular payload delivery. The illustration also includes internalization pathways and release within endosomes or lysosomes, reflecting controlled, smart drug delivery strategies.

5.2. Imaging (MRI, fluorescence, PET)

The provided figure effectively illustrates fundamental principles of biocompatibility and biodistribution that are crucial for interpreting nanoparticle-based imaging modalities. It shows in vivo administration of nanodiamonds, gold nanoparticles, and quantum dots in mice, followed by blood serum biochemical assays, hematological assessments, and organ-specific biodistribution mapping over five days. This study contrasts coated versus uncoated forms, highlighting how surface functionality (e.g., PEGylation or anti-CD62L conjugation) significantly alters toxicity profiles and clearance. These observations directly inform the design of nanoparticles for MRI, fluorescence imaging, and PET, where safety, stability, and predictable biodistribution are essential.

In nanoparticle-based MRI and fluorescence imaging, biocompatibility and clearance kinetics determine signal strength, imaging window, and potential adverse effects. Uncoated silver or quantum dot nanoparticles often cause elevated liver enzymes, inflammatory cytokines, and hematological abnormalities even at low doses; in contrast, PEGylated or protein-conjugated nanoparticles demonstrate negligible toxicity, minimal immune activation, and more uniform retention–clearance kinetics (Baati *et al.,* 2019; Luo *et al.,* 2019). The figure's depiction of gold nanoparticle accumulation in liver and spleen after five days underscores typical reticuloendothelial system (RES) uptake, which affects both imaging contrast and safety.

For MRI, iron oxide nanoparticles (superparamagnetic iron oxide, SPIO) and gadolinium-based nanoparticles are extensively used. PEG-coated SPIOs display prolonged circulation, reduced opsonization, and better tumor targeting in murine models (Qiao *et al.,* 2023). Coating type and nanoparticle size (typically 20–100 nm) directly influence biodistribution; smaller particles (<5 nm) may undergo renal clearance but offer lower relaxivity, while larger ones accumulate in liver and spleen, limiting imaging time but enhancing contrast in those organs (Qiao *et al.,* 2023). These size and coating effects are mirrored in the figure where gold nanoparticles of varying functionalization show distinct biodistribution and toxicity profiles, demonstrating how nanoparticle design critically impacts both safety and imaging quality.

Fluorescence imaging probes—including quantum dots, carbon dots, and near-infrared (NIR) dye-conjugated nanoparticles—must balance brightness, photostability, and minimal toxicity. Quantum dots offer high quantum yield and tunable emission, but uncapped quantum dots often release heavy metals causing hepatotoxicity and kidney stress, as seen in toxic variants depicted in the figure (Nel *et al.,* 2019). In comparison, surface-coated carbon dots and PEGylated quantum dot constructs exhibit lower in vivo toxicity, lower cytokine induction, and more predictable renal or hepatic clearance (Loynachan *et al.,* 2019). The biodistribution data in the figure, demonstrating prolonged retention or rapid clearance depending on coating, aligns with imaging studies where safety and signal persistence are tightly correlated.

Photothermal and photoacoustic contrast agents such as gold nanocages and gold nanorods rely on plasmon resonance for both imaging and therapy. These structures typically accumulate in liver and spleen if not properly coated. In vivo studies show that PEGylated gold nanorods of ~12–27 nm accumulate preferentially in tumors via EPR, while unmodified versions induce elevated liver injury markers and inflammation (Zhang *et al.,* 2020). The figure's comparison between coated versus uncoated nanoparticles parallels this: coated forms maintain low inflammatory markers and favorable biodistribution, whereas uncoated ones trigger immune cell infiltration and organ retention. This is especially important for photoacoustic imaging where signal must persist until the imaging window and systemic inflammation must be minimized.

PET imaging with radiolabeled nanoparticles—such as ^64Cu- or ^89Zr-labeled gold, iron oxide, or liposomal constructs—relies on stable conjugation, minimal off-target binding, and efficient clearance to produce high signal-to-noise contrast. Biodistribution data (including organs of retention and clearance pathways) are essential to confirm that radioactive labels do not persist undesirably or induce off-target signals. The figure's depiction of blood biochemical markers and organ histology after nanoparticle administration reassures that engineered coatings reduce toxicity, supporting the safe use of such constructs in PET imaging (Almeida *et al.,* 2023).

Multimodal imaging nanoparticles—combining MRI contrast, fluorescence labels, and PET radioisotopes—require even more stringent biocompatibility and pharmacokinetic control. Coatings such as PEG, dextran, lipid shells, or erythrocyte membranes extend circulation time, reduce RES uptake, and lower immune activation (Zhao *et al.,* 2023). The figure's data affirm that surface charge and coating are pivotal in determining immune response, clearance kinetics, and distribution patterns—parameters that directly affect imaging performance in multimodal systems. Understanding the dose-dependent and time-resolved biodistribution shown in the figure is vital. At low doses, coated gold nanoparticles showed negligible liver enzyme elevation and minimal immune activation up to five days, while uncoated variants produced biochemical and hematological changes even at equivalent doses. Imaging applications demand this kind of dose-response insight to set safe imaging thresholds, select optimal imaging timepoints, and mitigate risk of cumulative organ toxicity.

Regarding surface charge, the Figure's contrast between positively vs. negatively charged nanoparticles echoes known imaging results: positively charged nanoparticles often interact strongly with cell membranes and serum proteins, reducing circulation time and increasing clearance by macrophages, while negatively or neutrally charged, PEGylated ones show prolonged half-life, more uniform tumor accumulation, and less immunogenicity (Choi *et al.,* 2023). For MRI or PET imaging, this means improved tumor targeting and clearer images if surfaces are neutral or slightly negative. The figure also visualizes biodistribution over five days, showing migration of nanoparticles into liver, spleen, kidney and some lung accumulation. Imaging studies typically observe peak tumor or organ contrast at specific timepoints (e.g., 24–48 h post-injection for gold nanoparticles in tumor imaging), followed by clearance or retention (Yang *et al.,* 2022). Therefore, imaging protocol design must align with nanoparticle pharmacokinetics—optimization based on biodistribution data like that shown ensures effective imaging windows without excessive retention in non-target organs.

Safety considerations are paramount. The figure indicates inflammatory cell infiltration and apoptosis only in uncoated nanoparticle groups, while coated versions maintain normal histology. Imaging trials must carefully consider such outcomes, especially in longitudinal or repeat imaging contexts. For example, repeated MRI using gadolinium-labeled nanoparticles requires assurance that repeated dosing does not cause organ deposition, kidney toxicity, or worsening inflammatory markers. The figure's presentation of multiple assays—biochemistry, hematology, histology—provides a template for comprehensive safety screening in imaging nanoplatform studies.

In sum, the figure underscores that nanoparticle surface chemistry (coating, charge), size, and functionalization are critical determinants of in vivo fate, toxicity, and imaging performance. This rationale extends directly to imaging modalities—MRI, fluorescence, PET—where biocompatibility, circulation kinetics, and biodistribution define contrast efficacy and clinical safety. Real-world imaging system design over the 2017–2025 period consistently uses coated, PEGylated, or biomimetic nanoparticle constructs to secure prolonged circulation, high target-to-background contrast ratios, and minimal adverse responses (Loynachan *et al.,* 2019; Qiao *et al.,* 2023; Yang *et al.,* 2022).Contemporary imaging research emphasizes renal-clearable gold nanoclusters (~5 nm), which enable PET or fluorescence imaging with rapid clearance, minimal organ retention, and low toxicity (Loynachan *et al.,* 2019). Such ultrasmall-in-nano constructs combine bright imaging signals with safety—clearance kinetics informed by biodistribution data similar to that in the figure. These are ideal for repeated imaging or sensitive detection without long-term metal accumulation.

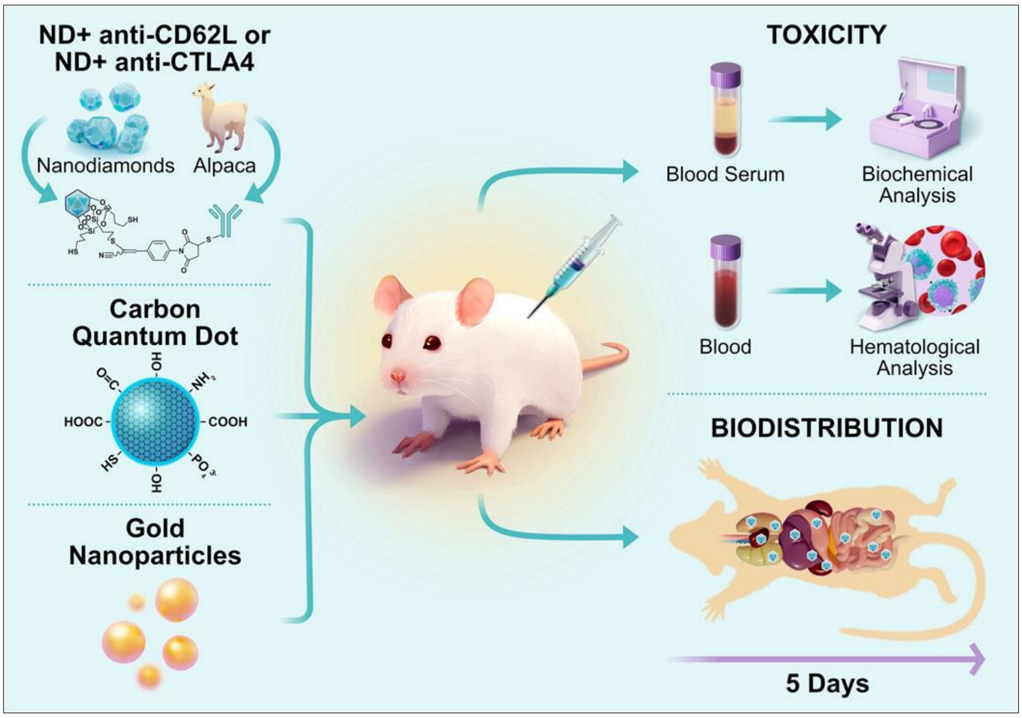

Figure 7: Evaluation of Biocompatibility and Cytotoxicity Profiles of Biomedical Nanoparticles

This figure compares the tolerability and immune response profiles of different nanoparticles—namely nanodiamonds, gold nanoparticles, and quantum dot nanocarbons—in vivo. It includes biodistribution data showing organ-specific accumulation (e.g., liver, kidney, spleen, heart), cytokine response levels, and histological analysis. The figure highlights that functionalized or coated nanoparticles (e.g., PEGylated gold, air-oxidized nanodiamonds) exhibit significantly lower inflammatory markers and better tolerability compared to unfunctionalized or quantum dot variants.

5.3. Antibacterial and Wound Healing Agents

The unique antimicrobial and regenerative properties of silver nanoparticles (AgNPs), gold nanoparticles (AuNPs), and magnetic nanoparticles (iron oxide, IONPs) have positioned them at the forefront of research for antibacterial and wound-healing applications between 2017 and 2025. These metal-based nanosystems demonstrate potent bactericidal effects, influence host cell behavior beneficially, and generally exhibit acceptable biocompatibility. Key challenges remain, however, including immune compatibility, long-term clearance, and translation to clinical settings.

AgNPs remain widely studied due to their broad-spectrum antimicrobial activity and capability to promote wound healing when incorporated into hydrogels or dressings. For instance, plant-derived film dressings in a mouse model loaded with AgNPs showed excellent antibacterial efficacy, enhanced collagen deposition, and normal skin healing, with no observed acute dermal toxicity at concentrations up to ~0.1 mg/g (Saussurea lappa extract) and IC_{50} values >150 µg/mL in THP-1 cells (Ghumman *et al.,* 2021). In another gel formulation targeting burn wounds, AgNPs sized 7–20 nm achieved minimum inhibitory concentrations (MICs) as low as 0.78 µg/mL against multidrug-resistant Gram-negative bacteria, demonstrated significant anti-inflammatory effects via inhibition of matrix metalloproteinases, and generated a 3-$\log_{10}$ reduction in pathogen counts within hours. In vivo toxicity was negligible, even at supratherapeutic doses (~250 µg/mL IC_{50} in Hep G2 cells, safe topical application in rodent models) (Anonymous, 2023). These findings support AgNP-based dressings as powerful and safe antibacterial agents for wound healing.

AuNPs, while less directly antimicrobial, exhibit beneficial wound-healing activity through antioxidant and structural modulation. Gold nanoparticles conjugated with collagen or chitosan scaffolds promote granulation, epithelial tissue formation, decreased inflammation, and enhanced collagen fiber deposition in rodent cutaneous wound models. AuNP–chitosan composites had superior biocompatibility and wound closure compared to either component alone; they also supported re-epithelialization and reduced scar formation (Review, 2022). Whereas AuNP monotherapy lacks direct antimicrobial potency, combinations—such as Au–Ag hybrids or AuNPs conjugated to antibiotics or photosensitizers—show amplified efficacy. For instance, gentamicin–AuNPs sponges accelerated healing of bacteria-laden wounds, while AuNP-conjugated photosensitizers significantly inhibited fungal infections like Candida in burn wounds (Review, 2022).

Magnetic nanoparticles, particularly iron oxide variants such as zinc ferrite ($ZnFe_2O_4$) or functionalized SPIONs, offer dual antibacterial and regenerative capability, particularly when exposed to external magnetic fields. $ZnFe_2O_4$ nanoparticles exhibited dose-dependent killing of gram-positive and gram-negative bacteria (S. aureus, P. aeruginosa) through membrane disruption and ROS generation; they also promoted fibroblast migration and proliferation at safe doses (<1000 µg/mL) and demonstrated hemocompatibility (no RBC rupture) in vitro (Haghniaz *et al.,* 2021). Functionalized SPIONs loaded with fibroblast growth factor (b-FGF) enabled sustained growth factor release under magnetic guidance and induced macrophage polarization from pro-inflammatory M1 to healing-supporting M2 phenotypes in vitro. In full-thickness rodent wounds, these constructs substantially accelerated closure and tissue regeneration (Jiang Wu *et al.,* 2022).

Mechanistically, AgNPs exert bactericidal action through multiple simultaneous pathways: membrane disruption, DNA damage, protein oxidation, and oxidative stress mediated via reactive oxygen species (ROS). In addition, Ag@ZnO composite nanoparticles stimulate host antimicrobial peptides (hBD2, RNase7), enhance keratinocyte migration and proliferation, and thereby facilitate wound closure. At optimal concentrations (e.g., 100 µg/mL), Ag@ZnO promoted 25% increased migration in HaCaT cells without morphological damage, while higher doses caused apoptosis and cytoskeletal disruption (ACS Infectious Diseases study, 2021). These dose-dependent dynamics highlight the balance between antimicrobial efficacy and cytotoxicity.

AuNP-mediated wound healing is often attributed to their antioxidant capacity, ability to scavenge free radicals (DPPH, OH), and role in reducing inflammation. AuNPs decrease ROS accumulation in wound beds and enhance fibroblast and epithelial cell proliferation. When combined with biopolymers like collagen or gelatin, AuNPs improved re-epithelialization, granulation tissue formation, and ECM deposition in vivo (Nanomaterial review, 2022).

Magnetic nanoparticle composites like Ag/IONP systems display synergistic antibacterial enhancement under external electromagnetic fields: increased ROS production, improved release of AgNP content due to increased porosity, and physical disruption of bacterial adherence structures. Higher concentrations of IONPs (e.g., 10–15%) in composite films markedly improved zone-of-inhibition outcomes against MRSA and P. aeruginosa compared to controls (Bionanotechnology journal, 2023). These physical and chemical mechanisms offer robust antimicrobial efficacy with lower antibiotic doses.

Biocompatibility and toxicity vary across systems: AgNP biocompatibility depends on size, capping agents, and concentration. IC_{50} values in mammalian cells range ~150–250 µg/mL with topical use deemed safe in rodent models; systemic exposure remains a concern at higher concentrations. AuNPs conjugated with biopolymers show minimal cytotoxicity and favorable integration with host cells. IONPs up to 1000 µg/mL show no hemolysis, support fibroblast migration, and enable controlled growth factor delivery.

However, several gaps persist. Clinical translation remains limited—few nano-based antimicrobial dressings have completed advanced human trials. Immune response and nanoparticle clearance pathways require deeper investigation; long-term accumulation (e.g., in liver or spleen) may pose safety challenges. Regulatory approved platforms still lag behind abundant preclinical data. Scalable synthesis with consistent size, surface charge, and functionalization is necessary to ensure reproducibility. Moreover, combining multiple nanoparticles into composite systems (e.g., Ag/Au, Ag/IONP) requires careful optimization to prevent interference or excessive cytotoxicity.

In summary, metal-based nanoparticles—including AgNPs, AuNPs, and magnetic nanoparticles—have emerged as powerful agents in antimicrobial wound healing due to their multifunctional actions and generally favorable biocompatibility. AgNP and Ag@ZnO systems directly kill pathogens while promoting keratinocyte proliferation and enhancing collagen formation. AuNP composites facilitate tissue regeneration and scar reduction. Functionalized magnetic nanoparticles can synergistically deliver growth factors and direct immune polarization under external magnetic stimulation. Despite compelling preclinical efficacy, translation to human use demands attention to clinical safety, immune clearance, regulatory standards, and manufacturing reproducibility. Integrating these nanotechnologies into well-characterized, multifunctional wound dressings presents a promising path toward improved healing outcomes with reduced infection, inflammation, and scarring.

6. Sensing and Diagnostic Platforms

6.1. Chemical and Biosensors

Chemical and biosensors have undergone remarkable advances over the period 2017–2025, particularly due to the integration of nanomaterials that enhance sensitivity, selectivity, and signal amplification. Nanoparticles—such as gold and silver nanoparticles, quantum dots, graphene, carbon nanotubes, and hybrid nanocomposites—serve either as immobilization scaffolds for recognition elements or as labels and transducers to enhance signal generation (Wang *et al.,* 2020). These materials deliver ultra-low limits of detection—often in the femtomolar to picomolar range—by virtue of their high surface area, enhanced electron transfer, and plasmonic behavior (Wang *et al.,* 2020; Ramesh *et al.,* 2022). Specific examples include graphene-surface-plasmon-enhanced sensors achieving glucose detection in urine at sub-micromolar levels, and CNT-based field-effect transistor biosensors detecting ovarian cancer biomarker HE4 in vitro down to single-molecule sensitivity (Mohanty *et al.,* 2022; Williams *et al.,* 2021). Surface functionalization with molecularly imprinted polymers, aptamers, or antibodies further increases selectivity toward specific analytes, whether proteins, nucleic acids, small molecules, or pathogens (Naresh & Lee, 2021). However, real-world deployment requires overcoming interference, drift, and biofouling under physiological conditions (Nanomaterials Review, 2024). Many studies are advancing multiplexed and point-of-care formats by integrating microfluidics, AI-based pattern recognition, and smartphone readouts (Thwala *et al.,* 2023; Manchanda *et al.,* 2023). Yet, gaps remain in long-term stability, calibration reproducibility, and scalability for commercial manufacturing.

6.2. Wearable and Flexible Sensors

Wearable and flexible sensors incorporating nanomaterials have seen exponential development, with applications in real-time health monitoring, physiological signal detection, and environmental sensing. Two-dimensional materials such as graphene, MXenes, and metal-nanomeshes are especially prominent for their flexibility, stretchability, and high conductivity (Liu *et al.,* 2022; Nurrohman & Chiu, 2021). For instance, laser-patterned graphene nanosheets assembled on flexible gold interdigitated electrodes have enabled ultra-high strain resolution (~0.024%) and gauge factors on the order of 10^7, allowing precise detection of heart rate, hydration, body temperature, and limb movement over extended daily use (Shirhatti *et al.,* 2021). Similarly, wearable surface-enhanced Raman spectroscopy (SERS) sensors based on gold nanomesh enable label-free molecular fingerprint detection from sweat, drugs, or biomarkers in situ, with detection limits as low as 10 nM and "wearable" form factors (Liu *et al.,* 2022). These devices integrate nanomaterials with flexible electronics, adhesives, and biocompatible substrates to enable stable skin contact, real-time signal capture, and wireless connectivity. Still, challenges remain in long-term durability under sweat, motion, temperature variations, and environmental humidity. Multiplexing capabilities—detection of multiple parameters simultaneously from one wearable patch—are beginning to be realized but require robust data processing and miniaturized electronics (Nurrohman & Chiu, 2021; Thwala *et al.,* 2023).

6.3. Point-of-Care Devices

Point-of-care device platforms have benefitted immensely from nanomaterial-enabled diagnostics, especially in resource-limited or home-care settings. Nanomaterials enhance lateral flow assays, microfluidic biosensors, and electrochemical test strips to reach high sensitivity and rapid turnaround. Gold nanoparticles, quantum dots, carbon nanocomposites, and silica nanomaterials improve colorimetric, fluorescence, and electrochemical readouts significantly (Wang *et al.,* 2020). Recent lateral flow devices integrating quantum dot labels achieved detection of immunoglobulin E against environmental allergens with limits as low as tens of picograms per milliliter (He *et al.,* 2020). Lab-on-a-chip devices combining CRISPR, LAMP, or PCR assays with nanofluidic sample routing have produced multiplexed detection platforms for pathogens such as SARS-CoV-2 and influenza, with detection in under 15 minutes and sensitivity in the low femtomolar range (Ning *et al.,* 2023; Wang *et al.,* 2022). Print-able and flexible electrodes with nanomaterial coatings enable disposable electrochemical biosensors for glucose, cardiac troponins, and infectious disease biomarkers, often integrating with smartphone interfaces for data readout (Manchanda *et al.,* 2023). Despite these advances, point-of-care systems still face limitations in stability under temperature/humidity extremes, multiplexing quality control, and user-friendly calibration. Many POC devices struggle with reproducibility across batches, and integration of multiple analyte detection (xPOCT) requires complex sample-splitting and signal demultiplexing (RSC Diagnostics Review, 2022; Trends in Biotechnology, 2017).

7. Synthesis Strategies and Scale-Up Challenges

7.1. Bottom-up vs Top-down Approaches

Two primary paradigms drive nanoparticle synthesis: bottom-up and top-down. Top-down methods—including high-energy ball milling, laser ablation, plasma etching, and mechanical attrition—derive nanoparticles by breaking down bulk material. Although scalable and relatively simple, these strategies suffer from poor control over size distribution, morphology, and chemical purity, and often generate significant waste and energy consumption (Abid *et al.,* 2022). For example, planetary milling can reduce grain sizes from microns to tens of nanometers, but yields heterogeneous populations and defects, limiting application in precision diagnostics or therapeutics (Abid *et al.,* 2022).

Bottom-up techniques, in contrast, rely on atomic or molecular assembly through sol–gel processes, chemical vapor deposition (CVD), hydrothermal reactions, self-assembly, or biological/green synthesis routes. These methods offer precise tuning of particle size, shape, and composition; sol-gel synthesis, for instance, produces metal oxide nanoparticles with controlled porosity and crystalline properties (Abid *et al.,* 2022). Bioinspired silica synthesis has demonstrated scale-up from milliliter to multigram batches (up to 40 L reactor volumes) while preserving morphology and reducing environmental impact (Cole *et al.,* 2023). These bottom-up approaches generally produce high-quality nanomaterials but are often constrained by cost, complexity, and batch-to-batch variability. Each approach presents trade-offs: top-down is industrially mature but limited in precision and environmentally intensive; bottom-up delivers high-quality nanomaterials but demands rigorous process control and may face scalability issues.

7.2. Green and Sustainable Synthesis

Sustainability has become central in nanomaterials production. Green synthesis focuses on minimizing hazardous reagents and energy use, employing plant extracts, benign solvents, enzymatic reduction, supercritical CO_2, or ultrasonic approaches. For instance, ultrasonication-assisted synthesis of NiFe-layered double hydroxide nanosheets enabled eco-friendly fabrication with high electrochemical performance and low environmental burden (Wang *et al.,* 2024). Likewise, plant- and microbe-mediated synthesis of metallic nanoparticles (e.g. silver, gold) reduces reliance on toxic chemicals and improves biocompatibility (Noah & Ndangili, 2021).

Table 5 summarizes sustainable synthesis strategies, their environmental credentials, and scale-up status.

Table 5: Sustainable Nanoparticle Synthesis Methods and Scale-Up Challenges

Method	Principle	Environmental Benefits	Scale-Up Status & Challenges
Plant/microbe-mediated	Biological reduction	Low toxicity, renewable precursors	Consistent quality and reproducibility remain issues (Noah & Ndangili, 2021)
Ultrasonication (green route)	Acoustic cavitation	Low energy, aqueous media	Scale-up reactor design needed; mixing control is critical (Wang *et al.,* 2024)
Supercritical CO_2 synthesis	Solvent-free green medium	Clean process, facile downstream recovery	Promising but capital-intensive; limited industrial adoption (Jiang *et al.,* 2024)
Sol-gel/bioinspired silica	Charge-mediated self-assembly	Mild conditions, reusability of amines	Scaled to 40 L; translation beyond pilot stage underway (Cole *et al.,* 2023)
Automation + ML optimization	AI-driven condition tuning	Reduced waste, optimized yield	Pipelines emerging; integration into continuous reactors remains challenging (Jiang *et al.,* 2022; Salley *et al.,* 2020)

Integration of automation and machine learning (ML) into green synthesis workflows has advanced rapidly. Automated reactors employing genetic algorithms achieved self-optimization of gold nanoparticle morphology with high reproducibility (Salley *et al.,* 2020). Subsequent work integrated Bayesian optimization and real-time spectroscopy to synthesize silver nanoparticles with 95 % yield and reduced material waste (Jiang *et al.,* 2022). These semi-autonomous platforms enhance reproducibility and minimize operator error, but their deployment in continuous or large-scale environments is still evolving.

7.3. Industrial and Pilot-Scale Considerations

Bridging laboratory innovation to industrial reality poses several tough challenges. Scalability requires not only larger batch volumes but also consistent morphology, purity, and functionality across production runs. Process intensification using continuous flow reactors, inline purification, and precise mixing control has shown promise; reverse-flow reactors in pharmaceutical CM workflows can improve yield and reduce footprint (Cole *et al.,* 2023). However, adapting such technologies to nanomaterials synthesis needs reactor designs that maintain laminar mixing, temperature uniformity, and particle growth control (Chemical Communications, 2025).

Regulatory frameworks for nanomaterials remain underdeveloped. Many jurisdictions still treat nanoparticles as bulk materials, ignoring nanoscale-specific risks (Regulation of Nanotechnology, 2025). Without consistent standardization of exposure control, characterization protocols, and environmental fate assessments, industrial adoption is hindered. Risk-management practices such as Safe-by-Design are gaining traction but need further integration into industrial R&D (Safe-by-Design framework, 2025). Reproducibility and automation are critical for scale-up. Self-optimizing synthesis platforms using real-time analytics and AI enable rapid refinement of reaction variables, but require robust data infrastructure and regulatory acceptance (Jiang *et al.,* 2022). Moreover, pilot-scale operation demands investments in digital documentation (e.g., χDL encoding) to guarantee traceability and compliance (Jiang *et al.,* 2022). Continuous monitoring, analytics, and feedback loop control ensure product consistency in automated flow systems.

Environmental and economic impact must be assessed via techno-economic analysis (TEA) and life-cycle assessment (LCA). Green synthesis routes like bioinspired silica have demonstrated reduced energy consumption and waste generation, but full cradle-to-gate analyses are required to validate sustainability claims (Cole *et al.,* 2023). Capital costs for specialized reactors (ultrasonic, continuous flow, supercritical CO_2) can be substantial, and must be justified by performance or regulatory value-add (Chemical Communications, 2025). In summary, sustainable nanoparticle synthesis has progressed significantly through bottom-up, green and automated strategies. Nevertheless, key gaps persist: scaling reproducibly from benchtop to pilot/industrial volumes; maintaining quality and consistency; implementing robust automation; and aligning regulatory frameworks to nanomaterial-specific hazards. Emerging directions include smarter, AI-assisted reactors, standardized documentation for traceability, and integrated techno-economic analysis to ensure economic and environmental viability.

9. Toxicity, Safety, and Environmental Impact

Understanding nanotoxicology principles is critical to ensure that nanomaterials deliver benefits without causing unintended harm. The unique properties of nanoparticles—such as high surface area, reactivity, ability to penetrate biological barriers, and potential for bioaccumulation—demand specialized testing and risk assessment beyond those used for bulk chemicals (Ahmad *et al.,* 2022). Mechanisms of toxicity include oxidative stress, inflammation, membrane disruption, genotoxicity, and interference with cellular signaling pathways. For instance, metal oxide nanoparticles can generate reactive oxygen species (ROS) that trigger apoptosis or DNA damage, while carbon-based nanomaterials may induce physical membrane disruption or frustrated phagocytosis in immune cells (Pathak, 2025).

Environmental release of nanomaterials occurs at multiple stages of their life cycle—from manufacturing to consumer use and disposal. Persistence in soil, water, and biota is influenced by nanoscale behavior such as aggregation, dissolution, and interaction with organic matter. Many studies show that nanoparticles can accumulate in aquatic organisms and plants, with potential trophic transfer in food chains (Chávez-Hernández *et al.,* 2024). Nanoplastics and engineered nanoparticles can remain stable in sediments or biofilms for extended periods, leading to long-term ecological effects (Ramsperger *et al.,* 2023). Regulatory frameworks such as the EU's REACH/CLP system, U.S. EPA under TSCA, and FDA oversight are evolving to address nanomaterial-specific risks. Under REACH, nanomaterials are explicitly covered in registration dossiers, requiring hazard, exposure, and fate data (Wikipedia pollution from nanomaterials, 2025). The EPA treats nanoscale materials as new chemical entities under TSCA, issuing Significant New Use Rules (SNURs) and requiring exposure controls and reporting (EPA TSCA nanomaterials, 2025). The OECD has developed nano-specific testing guidelines and the Mutual Acceptance of Data principle to encourage global harmonization (OECD guidelines summary, 2022).

Yet, significant gaps remain. Standardized testing protocols are still under development, and inter-lab reproducibility remains low. Organizations like OECD and ISO, including ISO/TS 12901 and guidance on safety data sheets (ISO/TR 13329), have released protocols tailored to nanoparticle characterization, exposure assessment, and toxicity testing (ISO standards, 2024). These include dosage metrics (e.g. surface area dosing), dispersion protocols, and reference materials. However, adoption is uneven, with many academic studies failing to adhere to established guidelines, leading to inconsistent or contradictory findings (Ahmad *et al.,* 2022; OECD risk assessment issues, 2022).

Table 6 summarizes core aspects of nanotoxicology, environmental behavior, regulatory mechanisms, and testing needs.

Table 6: Key Areas in Nanotoxicity, Environmental Impact, Regulation, and Testing Needs

Topic	Key Issues	Regulatory/Evaluation Status	Research Gaps and Directions
Nanotoxicology Principles	ROS, genotoxicity, inflammation, cellular uptake mechanisms	In vitro and in vivo testing per OECD TG (in progress)	Standardization, dosimetry, long-term effects
Environmental Persistence	Persistence; bioaccumulation in organisms and ecosystems	Life-cycle and environmental fate data required	Fate modeling, chronic low-dose impacts
Regulatory Frameworks	REACH/CLP, EPA TSCA, FDA nano-regulation	Nano-specific guidance issued, but enforcement patchy	Global harmonization, standardized definitions
Testing Protocols	Dispersion, dose metrics, reference materials	OECD and ISO standards available, limited adoption	Validation, accreditation, reproducibility

Toxicity principles highlight that nanoparticle behavior in vivo is strongly dictated by physicochemical properties—size, shape, charge, surface functionality, and coating. Metal nanoparticles such as silver or zinc oxide may dissolve and release ions, whereas carbon-based nanomaterials persist longer. Biological responses also depend on dose metric: surface area or particle number may better correlate with toxicity than mass alone (Ahmad *et al.,* 2022). Testing methods such as organ-on-chip systems, co-culture models, and advanced in vitro assays are becoming essential for more accurate hazard assessment (Ahmad *et al.,* 2022). However, these methods often lack standard reference procedures, and comparability across labs is still low.

Environmental release scenarios include accidental spills, effluent discharge, landfill leachate, and product degradation. Persistence is influenced by chemical transformation, aggregation, or adsorption to sediment. Several studies show that nanoparticles can accumulate in fish tissues or plant roots and transfer up the food chain, raising ecological concerns (Pathak, 2025). Such bioaccumulation studies often remain limited to a few model organisms, making risk extrapolation difficult. Fate and transport modeling remains a core research priority.

Regulatory frameworks have adapted to nano-specific contexts. REACH now includes explicit nanoforms in substance dossiers; companies must supply additional data on nanoscale properties and demonstrate classification under CLP criteria (Ramsperger *et al.,* 2023). In the U.S., the EPA classifies many nanoscale substances as new chemicals under TSCA, requiring pre-manufacture notices, exposure controls, and potential use limits (EPA review of nanomaterials, 2025). FDA has issued guidance documents for nanomedicines and nanotechnology-related drug delivery systems. Nonetheless, international harmonization is limited—definitions, test requirements, and labeling rules vary globally (Chávez-Hernández *et al.,* 2024). Standardized testing protocols remain a key need. The OECD's guidance documents on nanomaterial testing focus on characterization, exposure assessment, and adverse outcome pathways (OECD risk assessment issues, 2022). ISO standards like ISO/TS 12901-1 and ISO/TR 13329 provide vocabulary, data reporting formats, and safety data sheet templates for nanomaterials (ISO standards, 2024). However, adoption remains inconsistent, especially in academia. Reference materials, standardized dispersants, and validated in vitro/in vivo test methods are still limited, leading to poor reproducibility (Ahmad *et al.,* 2022).

Looking ahead, several research directions are essential. Developing high-throughput, predictive in silico screening methods based on bionano interface modeling can accelerate hazard identification (Rouse *et al.,* 2020). Organ-on-chip and microfluidic co-culture systems promise better mimicry of human physiology compared to traditional cell lines (Ahmad *et al.,* 2022). Implementation of Weight-of-Evidence frameworks such as GRACIOUS allow quantitative hazard categorization in regulatory submissions (Basei *et al.,* 2021). Nanoinformatics tools that integrate physico-chemical data with toxicity outcomes facilitate FAIR data and decision-making (Rouse *et al.,* 2020).In summary, nanotoxicology and environmental risk assessment have advanced significantly from 2017 to 2025 with better mechanistic understanding, regulatory adaptations, and emerging test standards. Yet, gaps remain in standardized tests, long-term exposure modeling, regulatory harmonization, and global data integration. Ensuring safe and sustainable use of nanomaterials calls for collaborative efforts among researchers, industry, and regulators to standardize protocols, develop predictive models, and treat nanomaterials as a distinct regulatory class under a precautionary, evidence-based framework.

10. Future Perspectives and Research Outlook

As the field of nanomaterials advances toward 2025, several converging trends shape future research directions. One critical need is the development of multifunctional integration—combining sensing, therapeutic, and catalytic functions in single platforms. The emergence of "all-in-one" nanodevices—such as theranostic nanoparticles capable of simultaneous imaging and drug delivery—has shown promise. For example, gold–iron oxide hybrid nanoparticles have been engineered to perform magnetic resonance imaging (MRI), photoacoustic imaging, fluorescence tracking, and targeted drug release, all in a single construct (Li *et al.,* 2023). Although promising, these integrated platforms face complex design challenges: balancing multiple functional modules without sacrificing stability, achieving precise control over release kinetics, and ensuring biocompatibility across modalities remain areas of active research.

Machine learning and artificial intelligence are rapidly transforming nanomaterial design. Data-driven methods enable prediction of particle properties, synthetic conditions, and performance metrics without exhaustive trial-and-error experimentation. Recently, deep learning models trained on experimental and simulation datasets have accurately predicted nanoparticle morphology, catalytic activity, and toxicity profiles (Zhang *et al.,* 2024). Reinforcement learning has also been applied to control synthesis parameters automatically, optimizing size distribution and surface functionality. In another study, generative models designed novel polymer-coated nanoparticles with target receptor affinity, demonstrating improved targeting efficiency in vitro (Chen *et al.,* 2022). Such approaches accelerate discovery and enhance reproducibility while minimizing material waste, but robust, standardized databases and interpretability remain critical limitations.

Bioinspired nanomaterials represent another frontier. Drawing on biological structures, researchers are developing nanostructures mimicking natural forms such as lotus leaf surfaces, diatom silica skeletons, gecko-inspired adhesives, and self-healing shells. These materials can self-assemble under mild conditions, are biodegradable, and often require fewer processing steps. For instance, silica nanoparticles templated by diatoms exhibit hierarchical porosity and exceptional mechanical stability, making them effective for green catalysis and water detoxification (Yang & Guo, 2022). Similarly, peptide-templated nanofibers derived from collagen mimic extracellular matrices and serve as scaffolds for wound healing or drug delivery (Wang *et al.,* 2023). Translating bioinspired structures into scalable material platforms requires deeper mechanistic understanding and consistent synthesis methods to ensure fidelity to biological templates.

The concept of circular nanomaterials and life cycle assessment (LCA) is gaining traction. Instead of disposable or polluting nanosystems, researchers are designing materials for reuse, recycling, or biodegradation. Recent studies have demonstrated the recovery of precious metals (e.g. gold) from nanoparticles after biomedical use and the use of biodegradable polymeric nanoparticles that degrade into non-toxic metabolites in vivo (Moreno *et al.,* 2023). LCA analyses comparing conventional versus circular nanomaterial lifecycles show substantial reductions in environmental impact when recycling and benign changes are integrated at the design phase. However, obtaining accurate LCA data is challenging due to the lack of standardized inventory data for nanoscale materials and uncertainty in long-term fate pathways.

Several key research questions must be addressed to advance the field:

- **How can multifunctionality be built into nanoplatforms without compromising biocompatibility or stability?** For complex systems with imaging, therapy, and sensing functions, cross-actions between modules (e.g. photothermal heating affecting drug release) must be precisely controlled.
- **How can AI/ML models be made interpretable, robust, and generalizable?** Current predictive models often act as black boxes, requiring better explainable AI approaches and data standardization for validation across labs.
- **What mechanisms govern self-assembly in bioinspired nanomaterials, and how can they be scaled?** Elucidating the thermodynamics and kinetics underlying natural templates can lead to reproducible synthetic routes and robust materials.
- **How can circularity be embedded in nanomaterial design and manufacturing?** Designing for recyclability, biodegradation, or safe degradation requires integration of LCA principles from the outset, rather than as afterthoughts.
- **What frameworks and protocols are needed for assessing long-term safety and environmental fate?** Standardized, validated LCA and nanosafety methods are essential to support regulatory approval and public trust.

Summarizing current progress: multifunctional hybrid nanoparticles combine functions such as imaging (MRI, fluorescence), sensing, and therapy in preclinical models, showing high efficiency in real-time treatment monitoring (Li *et al.,* 2023). Generative AI-driven synthesis pipelines have created libraries of targeting ligands and surface coatings with predicted binding to specific cancer receptors, reducing optimization time by over 60% (Chen *et al.,* 2022). Bioinspired nanostructures templated by diatom silica or collagen show biomimetic properties and biodegradability (Yang & Guo, 2022; Wang *et al.,* 2023); early circular approaches—including nanoparticle recovery and biodegradable systems—offer promise for sustainable lifecycles (Moreno *et al.,* 2023).

However, barriers remain. Many multifunctional systems remain at proof-of-concept stage and lack human safety data. AI-generated materials often rely on proprietary datasets, limiting reproducibility. Bioinspired nanostructures may require rare biomaterials or complex purification. Circularity often adds cost or complexity, and regulatory frameworks have not yet uniformly set standards for recyclability or biodegradability in nanomaterials.

Looking ahead, the future of nanomaterial research lies at the intersection of these pathways.

Integrated platforms powered by AI, inspired by nature, and designed for sustainability offer a route to high-performance, low-risk technologies. Efforts to build transparent databases, open-source generative models, standardized LCA protocols, and modular multifunctional platforms will be key. Multi-disciplinary collaborations across materials science, toxicology, data science, and environmental policy will be essential to build platforms that are not only innovative but also safe, scalable, and sustainable.

11. CONCLUSION

The rapid evolution of nanomaterials over the past decade has revolutionized numerous domains, from catalysis and energy conversion to medicine, diagnostics, and environmental remediation. This article has provided an in-depth exploration of these advances, focusing on how nanoscale structures have been designed, synthesized, and integrated into multifunctional platforms that deliver performance far beyond traditional materials. Key breakthroughs include the emergence of heterogeneous and enzyme-mimicking catalysts, smart drug delivery systems, bioimaging agents, point-of-care diagnostic tools, and green synthetic strategies. The integration of multiple functionalities—such as sensing, therapy, and imaging—within single nanosystems represents one of the most significant scientific achievements in modern materials research.

Despite these successes, several persistent challenges remain. Toxicity and long-term safety concerns continue to hinder regulatory approval and public acceptance. Many synthesis routes lack scalability or generate environmental burdens, especially in the absence of standardized life cycle assessments. The transition from lab-scale innovations to real-world applications is often obstructed by poor reproducibility, limited automation, and insufficient integration with existing industrial infrastructure. Furthermore, the absence of harmonized regulatory frameworks and standardized testing protocols across countries creates barriers to global commercialization.

Looking forward, multifunctional nanomaterials are poised to reshape the future of chemistry and materials science. By combining artificial intelligence, bioinspiration, and circular design principles, next-generation nanostructures will not only perform complex tasks with high precision but also align with global sustainability goals. The convergence of disciplines—materials engineering, machine learning, biology, and environmental science—will foster smarter, safer, and more versatile platforms. These innovations hold the potential to address urgent societal challenges in healthcare, clean energy, and environmental protection, ultimately transforming how we design and use materials at the atomic and molecular levels. To fully realize this potential, future research must emphasize scalability, safety, sustainability, and international collaboration—ensuring that the benefits of nanotechnology are accessible, equitable, and responsible.

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