Journal of Chemical Reviews
2026, Volume 8, Issue 2

Review Article

A Comprehensive Review of Heavy Metal Contamination and Sustainable Nanomaterials in Environmental and Economic Considerations

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Citation: B. Venkatesh, K.K. Saxena, N.D. Raja, A. Kumar, R. C., V. Sivasundar, B. Challa, P. Satishkumar, L. Sehgal, **A Comprehensive Review of Heavy Metal Contamination and Sustainable Nanomaterials in Environmental and Economic Considerations**. *J. Chem. Rev.*, **2026,** *8*(2), 241-268.

https://doi.org/10.48309/JCR.2026.539008.1490

ARTICLE INFO

Received: 2025-08-04
Revised: 2025-10-06
Accepted: 2025-10-30
ID: JCR-2508-1490

Keywords:
Sustainable nanomaterials, Mechanisms of heavy metal removal, Synthesis, Life cycle assessment, Recent innovations

ABSTRACT

Human-made processes were causing severe heavy metal contamination in surface waters, creating more health hazards in industrial development. Nanomaterials have advantages because they possess larger surface areas, organic properties, and comply with ecologically friendly production standards. In this study, the heavy metal remediation was explored through the examination of bio-based nanostructures and hybrid nanomaterials. The present study discusses metal efficiency in terms of decomposing the removal mechanisms that involve plant extracts, microbial pathways, and also life cycle assessments, as well as the economic needs necessary to sustain long-term operations. Recent advances in smart nanomaterials based on bio-hybrid systems and multifunctional nanocomposites have defined the new trends that shape the materials sector. This study is a review article that considers the potential of sustainable nanomaterials in the remedial process of heavy metals to devise the optimal methods of synthesis and ensure sustainable industrial utilization of the synthetic materials in environmental cleanup.

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1. Introduction

Sustainable nanomaterials present a promising solution that helps to solve various energy-related and information technology-based environmental and health-related problems. These materials are designed using renewable and natural resources with minimal impact on society, integrating sustainability with nanotechnology to optimize performance [1].
The development of sustainable nanomaterials aims to maximize the benefits of nanotechnology while minimizing undesirable impacts on health and the environment [2]. While nanomaterials offer numerous advantages, there are concerns about their potential impacts on health and the environment [3]. The nanomaterials serve as a vital solution to challenge numerous industry matters, as safety receives methodical evaluation with sustainability elements during design [4-7].
Heavy metal contamination endures as a major environmental problem that affects across extensive worldwide areas be due to industrial and rapid population growth [8,9]. These metals exhibit the non-degradable behavior, leading to the gradual accumulation in the environment [10]. The occurrence of excessive amounts of metals causes detrimental effects on wildlife [11-14] and also shows conflicting effects on health because chromium behaves differently when it exists as Cr^{6+} and Cr^{3+}.

2. Types of Sustainable Nanomaterials for Heavy Metal Removal

Different types of nanomaterials, such as carbon nanotubes, graphene, and graphene oxide, demonstrate top-level abilities to extract heavy metals [15,16]. These materials are presented in abundant active areas and functional improvements, which increase collection competence and absorption capacity [17]. Researchers discovered nanocomposites and metal-oxide nanomaterials used as adsorbents [18,19].
Polymer-supported nanoparticles exhibit notable selectivity and demonstrate high capacity for heavy metal ion removal[20-22]. **Tables 1** and **2** show the types, applications, and the latest literature reviews for sustainable nanomaterials.

3. Mechanisms of Heavy Metal Removal Using Nanomaterials

3.1. Adsorption mechanisms

This mechanism evolves based on the specific adsorbate-adsorbent pair and the surrounding conditions of the environment. The adsorption behavior of catechol on goethite occurs through mononuclear monodentate and binuclear bidentate configurations but the adsorption mechanism depends on pH along as well as surface coverage conditions [73,74].

Table 1. Types and applications of nano materials

Type of nano material	Examples and composition	Applications	Ref.
Carbon-Based nanomaterials	Graphene, carbon nanotubes (CNTs), Activated carbon, biomass, coal, and coconut shells	Heavy metal adsorption, wastewater treatment, and filtration membranes	[23-28]
Metal and metal oxide nanoparticles	Fe_3O_4, Fe_2O_3, zinc oxide TiO_2, AgNPs Fe, Zn, Ti, and Ag synthesized via green	Heavy metal removal, photocatalysis, and antibacterial coatings	[29-35]
Biopolymer-Based nanomaterials	Chitosan, cellulose nanofibers, starch-based nanoparticles, chitin, plant fibers, and starch	Water purification, biomedical applications, and food packaging	[36-39]
Clay and zeolite-based nanomaterials	Montmorillonite, kaolinite, and zeolites	Removal of heavy metals, soil remediation, and catalysis	[40-44]
Waste-Derived nanomaterials	Fly ash-based nanomaterials, agricultural waste-derived nanoparticles (rice husk and banana peel), and industrial/agricultural waste converted into nanomaterials	Heavy metal adsorption and environmental remediation	[45-52]
Hybrid and composite nanomaterials	Metal-organic frameworks (MOFs), graphene-based composites, polymer-nanoparticle hybrids, and mixture of organic and inorganic materials	Advanced water treatment, gas separation, and sensing applications	[53-59]

Table 2. The summery of previous works

Sr./ No.	Title of the article	Description	Year of publication	Ref.
1.	Innovative approaches in nanomaterials for efficient heavy metal removal from wastewater: A scientific review	This work studied the application of adsorption produced new opportunities through recent nanotechnology developments in high-performance nano adsorbent and also this paper examines TiO_2, Fe_3O_4, carbon-based materials and polymeric nanocomposites, explaining the porous structure effects alongside functional group behavior.	2024	[60]

2.	Nano-revolution in heavy metal removal: Engineered nanomaterials for cleaner water	This study explains the nanomaterial functionalization to boost material separation efficiency, along with stability and expanding adsorption capacity. The adsorption process mainly depends substantially on experimental conditions that include temperature, adsorbent level, pH, and ionic strength.	2024	[21]
3.	Nanomaterials for efficient removal of heavy metals	This research discusses four different nanomaterials on heavy metals efficiently and also explains fundamental mechanisms of nanomaterial-heavy metal ion reactions through descriptions of adsorption, ion exchange and surface complexation processes. The article evaluates nanomaterial-based remediation challenges, emphasizing the necessity of designing remediation systems properly.	2023	[61]
4.	Heavy metal removal from aqueous effluents by TiO_2 and ZnO nanomaterials	This work focuses on metal oxide semiconductor nanomaterials because these materials demonstrate high efficiency in water purification by driving the photoreduction of ions after they absorb suitable wavelength light. This research evaluates existing studies about nanomaterial adsorption and photocatalysis, focusing on major physical factors affecting these processes.	2023	[62]
5.	Sustainable use of nano-assisted remediation for mitigation of heavy metals and mine spills	This review investigated present trends and identified necessary improvement areas before discussing the need for inter-disciplinary nanotechnology applications in deploying multi-purpose remediation treatments across different contaminants.	2022	[63]
6.	Function of nanomaterials in removing heavy metals for water and wastewater remediation: A review	The objective of this paper was to analyzed how synthesized nano adsorbents function in heavy metal ion cleansing from water bodies and wastewater, together with their capability to increase adsorption strength and separation effectiveness.	2022	[64]
7.	Nanocellulose-based adsorbents for heavy metal ions	The utilization of nanocellulose-based adsorbents as environmentally friendly materials for heavy metal removal relies on their three key attributes.	2022	[65]
8.	Dodonaea angustifolia Extract-Assisted Green Synthesis of the Cu_2O/Al_2O_3	The researchers combined the coprecipitation synthesis method for producing Al_2O_3 and Cu_2O nanoparticles using D. angustifolia plant extract	2023	[66]

	Nanocomposite for adsorption of Cd(II) from Water	before preparing. The adsorption isotherm data showed the most suitable fit with the Langmuir adsorption model and pseudo-second-order kinetic model while achieving a maximum adsorption capacity of 4.48 mg/g.		
9.	Advances on ZnO hetero-structure as a nanoadsorbent for heavy metal removal	The research community has centred on nano-adsorbents for their unique characteristics that make them suitable for heavy metal removal from water over the past ten years. This chapter presents information about the synthesis procedure for ZnO NPs alongside their nanocomposite production and also provides an extensive analysis of ZnO-based nanostorbents.	2023	[67]
10.	Utilization of biosynthesized silica-supported iron oxide nanocomposites for the adsorptive removal of heavy metal ions from aqueous solutions	The research examines heavy metal ions extraction from simulated water through the use of biosynthesized silica-supported iron oxide nanocomposites (nano-IOS). Fabrication of nano-IOS occurs through an eco-friendly method using agricultural wastes as raw materials. The adsorption process of nano-IOS followed the Langmuir adsorption isotherm and pseudo-second-order kinetic model, which demonstrated chemisorption on the surface of nano-IOS.	2022	[68]
11.	Recent Advances in Adsorptive Nanocomposite Membranes for Heavy Metals Ion Removal from Contaminated Water: A Comprehensive Review	This review investigates extensive details about modern nanomaterial-based approaches in nanoadsorptive membrane systems to treat wastewater while removing heavy metals and also examines how the relevant characteristics of nanostructures influence their performance for water treatment and contamination elimination processes.	2022	[69]
12.	Removal of Toxic Metals from Water by Nanocomposites through Advanced	Research shows heavy and toxic metals are increasingly present in global water sources, leading to severe effects on human health and ecosystems. Research activities in recent times	2023	[70]

	Remediation Processes and Photocatalytic Oxidation	have produced advanced nanostructures that demonstrate remarkable abilities regarding heavy/hazardous metal adsorption while simultaneously achieving metal ion photo-degradation capabilities. Nanoparticles offer controlled physical and chemical modifiable characteristics. The review evaluates how carbon-based nanomaterials, polymer-based nanomaterials, and semiconductor-based nanomaterials can be used for adsorption.		
13.	Tuning phase compositions of MoS_2 nanomaterials for enhanced heavy metal removal: performance and mechanism	Two phases of MoS_2 materials were synthesized through hydrothermal reactions to obtain morphologically comparable solids that differed mainly by their physical characteristics. Results demonstrated that 1T-MoS_2 performed better in capturing Ag^+ and Pb^{2+} cations than 2H-MoS_2. The Pb^{2+} adsorption capacity of 1T-MoS_2 samples reached ~632.9 mg g-1, which represented an eight times greater performance than the 2H-MoS_2 samples, which had ~81.6 mg g-1 capacity.	2022	[71]
14.	Nanomaterials for the removal of heavy metals from wastewater	Nanotechnology functions as an upcoming technology that draws rising attention, while scientists have created various nanomaterials to detoxify heavy metals in polluted water supply sources.		[72]

The adsorption behavior of ligands on gold nanoparticles shows positive or negative cooperative effects because different nanoparticle facets exhibit different adsorption patterns. Scientists can use this mechanism to control facet development during the synthesis of colloidal metal nanoparticles. During the adsorption process, thermal activation plays a crucial role in determining the speed at which reactions occur, while equilibrium and non-equilibrium components work together [75-82]. **Figure 1** displays the adsorption, absorption, and sorption mechanisms. **Table 3** shows the comparative efficiency data for different metals and **Table 4** mentions case studies of AI and ML integration.

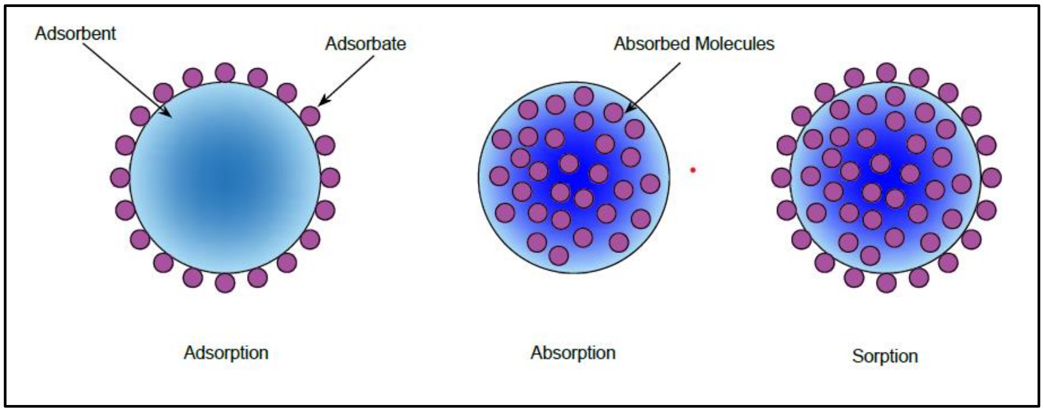

Figure 1. Adsorption, absorption, and sorption mechanisms

3.2. Absorption mechanisms

The specific mechanisms used for absorption differ based on the type of substance and the living organism. The absorption of thyrotropin-releasing hormone (TRH) occurs through carrier-mediated transport in the upper part of the small intestine [83]. This mechanism displays saturation characteristics while, oligopeptides and antibiotic inhibitors validate the existence of specific transport channels. The absorption of volatile compounds from tap water occurs through several entry pathways, including consumption, breathing and skin contact. Risk assessment assumptions become more accurate when researchers incorporate data about how showering boosts chemical body accumulation through the nose and skin pathways [84]. These mechanisms are influenced by various factors, including phytohormones, microRNA, root development, and mycorrhizal symbiosis [85]. In the case of heavy metals, absorption can occur through ingestion or other routes, with accumulation rates often exceeding discharge rates, leading to toxicity [86]. Understanding these diverse absorption mechanisms is crucial for improving nutrient use efficiency in plants, assessing environmental risks, and developing strategies to mitigate the harmful effects of toxic substances.

3.3. Ion exchange

The ion exchange operations within nanomaterials serve as vital elements to control atomic-level composition, along with interface and morphology. Material perfection becomes possible through this process despite traditional synthesis methods offering limited control [87]. Both anion and cation exchange reactions exist in II-VI and III-V semiconductor magic-size clusters. These reactions serve two purposes: they enable the design of complex MSCs and reveal mechanisms by which ions enter nanocrystals [88]. For semiconductor colloidal nanocrystals, cation exchange proceeds rapidly and reaction thermodynamics are modifiable through solution-based selective ion coordination. The solution allows the synthesis of nanocrystals that conventional methods cannot produce due to their unorthodox compositions, morphologies and crystal phases [89]. The surface crystal facets also play an important role during the ion exchange process. Rapid ion exchange occurs in rock salt PbTe nanocrystals with cuboctahedral shapes due to the presence of both neutral {100} and polar {111} facets. In contrast, cubic nanocrystals with only neutral facets do not react because of their lack of polar surfaces. The main reason behind this observation relates to the differing surface areas between {111} facets that accelerate the exchange process [90]. The processes of ion exchange in silicate glasses occur when oxygen ions on silicon oxygen tetrahedra exchange Na^+ and H^+. The transport of water through metal halide perovskite nanostructures happens after surface reactions through clustered non-bridging oxygen exchange reactions assisted by water molecules [91] .

3.4. Redox reactions

Nanomaterial behavior, along with its practical applications, heavily depends on redox reactions. Electron transfer occurs between species during such reactions, which affects the oxidation states of the involved species. In nanomaterials, redox reactions can significantly impact their properties, structure, and functionality [92,93]. For instance, in bimetallic nanoparticles, redox reactions can drive structural and compositional changes, affecting their catalytic performance. Similarly, the redox properties of CeO_2 nanoparticles, attributed to their Ce^{3+}/Ce^{4+} ratio and oxygen vacancies, contribute to their antioxidant and enzyme-mimicking activities [94]. The redox behavior of nanomaterials can be both beneficial and potentially harmful. While some nanomaterials act as strong antioxidants, scavenging reactive oxygen species (ROS), others may promote ROS generation, potentially leading to oxidative stress [95]. This dual nature is exemplified by MXenes, which can be utilized for both pro-oxidation and anti-oxidation processes in various biological applications [96]. Additionally, the redox reactions in nanomaterials can be influenced by external factors such as electron beam irradiation in liquid-cell transmission electron microscopy, affecting the dynamics of the system [97-100].

3.5. Chelation and complexation

The process of heavy metal elimination through nanomaterials relies on chelation combined with complexation functions. Nanomaterial functionality works through the formation of molecular bonds between surface groups and metal ions, which provides effective wastewater and soil contaminant removal capabilities. Among these nanomaterials, functionalized graphene oxide and metal-organic frameworks use chelation as their primary heavy metal removal method. Nanotech researchers synthesized a chelating membrane containing sulfonated graphene oxide and metal-organic frameworks to remove Cu^{2+} and Pb^{2+} with 99.4% efficiency in two hours [101]. Simultaneously, phosphonate-functionalized layered cationic frameworks demonstrated high affinity for Zn^{2+} (281.36 mg/g) and Fe^{3+} (206.03 mg/g) through chelative adsorption [102]. The chemical modification of cellulose creates binding sites that produce enhanced reactivity, enabling different removal strategies such as ion exchange, electrostatic interactions, complexation, and chelation [103]. The core-shell Fe_3O_4@SiO_2 nanoparticles containing iminodiacetic acid chelators called FS@IDA represent a powerful magnetic solid chelator that both separates non-magnetic heavy metals from the soil by chelation and performs efficient magnetic separation processes [104,105].

3.6. Surface functionalization and modification

These techniques enhance adsorption ability and the stability of nanomaterials, resulting in more effective contaminated water treatment [21,101,105]. **Figure 2** shows the surface functionalization and modification process. Research shows that iron oxide nanoparticles undergo functionalization processes to boost their ability to extract heavy metal ions from aqueous systems [106]. Many studies focus on emerging oxide nanomaterials, including ZnO, Fe_3O_4, and TiO_2, along with their nanocomposites through surface modifications to enhance their sorption abilities for removing heavy metal ions and organic dyes [107]. The grouping of materials through surface modification techniques recovers many characteristics while achieving integrated detection and removal functions. Nanomaterial effectiveness during removal processes depends on several conditions, which include pH concentrations, dosage amounts, temperature measurements, and contact durations, along with ionic strength measurements.

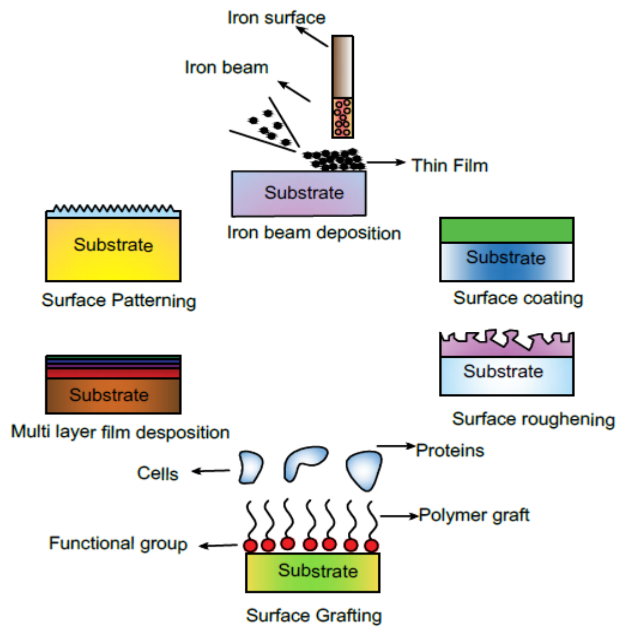

Figure 2. Surface functionalization and modification process

Table 3. The comparative efficiency data for different target metals across each removal mechanism

Mechanism	Removal efficiency / Capacity	pH	Scalability	Environmental impact	Ref.
Adsorption (activated carbon, biochar, and composites)	Pb (II): 95–99%, q_{max}: up to 250 $mg{\cdot}g^{-1}$; Cd (II): 80–92% and q_{max} ~110 $mg{\cdot}g^{-1}$)	5–6	High	Disposal of used adsorbents may generate secondary waste.	[108]
Ion exchange (zeolites and synthetic resins)	For Cu(II), Zn(II) metals, and Pb(II) Removal 70–95%; exchange capacity 1.0–1.5 $meq{\cdot}g^{-1}$	4–6	Moderate	Potential leaching of chemicals during regeneration may pose risks	[109]
Chelation/complexation (EDTA and iminodiacetic resins)	For Cd(II), Ni(II), Pb(II) metals, and Complexation efficiency ~85–95%;	5–7	Moderate	Possible nanoparticle aggregation and toxicity to aquatic organisms	[110]
Surface modification (thiol, amine, and magnetic functionalization)	Hg(II): up to 99% and q_{max} > 300 $mg{\cdot}g^{-1}$; Pb(II): 90–98%	4–6	Moderate	Eco-friendly, biodegradable pathways reduce long-term risks	[111]

4. Synthesis of Sustainable Nanomaterials

4.1. Green synthesis approaches

Sustainable nanomaterial synthesis methods based on green approaches have received substantial interest because they produce lower-toxicity particles while using less energy and lowering production expenses compared to conventional methods [112]. Biomolecules and phytochemicals extracted from plants and microbes function as reducing and stabilizing agents for nanoparticle synthesis while meeting the global demand for environmentally friendly processes [113]. The green synthesis of nanoparticles relies on biological agents such as bacteria, yeasts, fungi, algae and plant extracts [114]. The pharmaceutical components within Cannabis sativa L. demonstrate promise as silver nanoparticle synthesizing agents that find modern applications in medical science and pollution clean-up operations [115]. Research shows that fabricating zinc oxide-silver nanoparticles with strong antibacterial and anticancer properties can be achieved through Punica granatum fruit peel extract [116]. Green synthesis methods have various benefits but researchers must address three main obstacles: comprising low quantum yield, reproducibility difficulties, and ease of scaling [117]. However, integrating green chemistry principles and Safe and Sustainable by Design (SSbD) innovations can help overcome these limitations, paving the way for more consistent and scalable production of nanomaterials. Green synthesis approaches represent a promising avenue for sustainable nanomaterial production, offering a wide range of applications, from environmental remediation to cancer treatment, while minimizing environmental impact [118]. As research in this field progresses, standardization and continued innovation in synthesis methods are crucial for fostering the widespread adoption of green chemistry in nanotechnology [119].

4.2. Eco-friendly fabrication techniques

One of the main applications of green synthesis focuses on environmentally-friendly fabrication of nanomaterials which provides multiple benefits compared to traditional preparation methods. A wide range of nanomaterials, including metal and metal oxide nanoparticles, are synthesized through the green synthesis method with natural components such as plant extracts, bacteria and fungi [118]. The process uses biological components along with phytochemicals such as flavonoids, alkaloids, and terpenoids to function as reducing agents and solvents because they eliminate toxic chemicals [116]. Various eco-friendly fabrication techniques exist for developing sustainable nanomaterials. The combination of zinc oxide-silver nanoparticles (ZnO-Ag-NPs) was achieved through Punica granatum fruit peel extract as both the natural reducing and stabilizing agent, while nickel cobaltite nanoparticles ($NiCO_2O_4$ NPs) synthesized by using Hyphaene thebaica extract [113,120,121]. The utilization of green synthesis methods leads to nanoparticles with both improved environmental friendliness and increased functionality while minimizing ecological harm.

4.3. Waste-derived nanomaterials

Waste-derived nanomaterials constitute a promising method to produce sustainable nanomaterials that harmonize with green chemistry and the circular economy framework. The steps for waste-derived nanomaterials are shown in **Figure 3**. These materials enable sustainable synthesis of nanomaterials through substituted toxic chemical processes, which also minimize energy consumption [45,122]. Waste materials contribute several benefits to nanomaterial synthesis. The synthesis of efficient nanomaterials becomes possible through algae living cells because algal extracts contain reducing substances, stabilizing agents, and capping agents, which enable efficient synthesis [123]. Plant flowers feature multiple secondary compounds, which prove effective reducing agents in generating different metal or

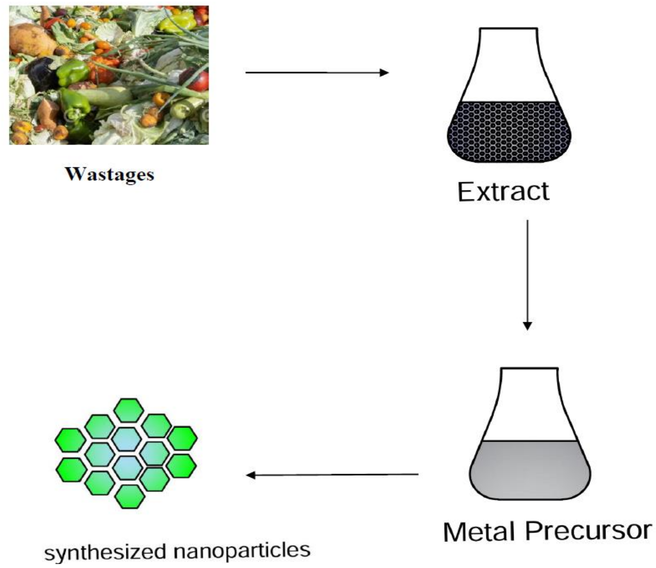

Figure 3. Steps for waste-derived nanomaterials

metal oxide nanoparticles [124]. Green materials and entities are used in production operations to determine the physical characteristics, the chemical reactions, and the biological system properties of nanomaterial end-products. The selection of waste-derived precursors creates new possibilities to customize nanomaterial properties. The incorporation of nanomaterials originating from waste into green supply chains fuels sustainability while creating innovative opportunities and securing lasting economic prosperity.

5. Environmental and Economic Considerations

5.1. Life cycle assessment (LCA) of nanomaterials

A comprehensive Life Cycle Assessment (LCA) enables researchers to assess the environmental impacts that nanomaterials generate throughout their complete life cycle. The assessment of nanomaterials via Life Cycle Assessment encounters various execution barriers. Research conducted on 71 studies spanning from 2001 to 2020 demonstrated poor completion of full LCA investigations for nanomaterials, especially at their end-of-life phase, thus producing uncertain results [125]. Future research on nanomaterial LCA should enhance data transparency by providing detailed life cycle inventory reports along with whole-life-cycle environmental impact assessments, transparent modeling approaches, complete risk, uncertainty, and sensitivity research. Nanomaterials create a minimum of three major obstacles when applied to current LCA assessment methods [126]. The emergence of nanotechnology has outpaced the acquisition of environmentally relevant data, making it difficult to integrate risk analysis (RA) and LCA based solely on dataset completion [127]. Additionally, the use of nanoscale silver in consumer products has raised concerns about potential environmental impacts as production demands increase [128]. To enhance the sustainability assessment of nanomaterials, it is recommended to apply both LCA and RA methods in parallel, integrating results after obtaining separate analyses. The environmental performance of nanomaterials can be improved through product stage life-cycle thinking, along with life-cycle and risk analysis integration and sustainable manufacturing methods combined with green chemistry alternatives [129].

Nanosilver in textiles shows high uncertainty due to nanoparticle release during washing, while TiO_2 photocatalysts demonstrate environmental benefits but require high energy for synthesis. Carbon nanotubes and graphene oxide exhibit significant energy and chemical demands, questioning sustainability. Similarly, ZnO nanoparticles, despite widespread use, contribute notable environmental impacts from energy-intensive production.

5.2. Environmental sustainability and economic viability

Nanomaterials provide significant environmental sustainability and economic viability options through applications in biofuel production, pollution removal, and green supply chains. The full-scale adoption of nanomaterials faces major obstacles due to the effectiveness and scalability demands. Nanomaterials serve as powerful tools for enhancing efficiency and decreasing environmental impact in manufacturing biofuels from lignocellulosic materials. Economic factors become essential since the proper evaluation of nanomaterial-related costs in biofuel manufacturing remains vital [130]. The process of environmental remediation benefits from metal oxide-based nanoparticles, which demonstrate excellent performance in pollutant removal. Cost-effectiveness and scalability represent major difficulties when the successful implementation of these nanoparticles occurs [131]. Various methods attempt to solve these existing difficulties. Unmodified iron oxide nanoparticles (BIONs) present a production method that reduces environmental impact, enhances scalability benefits, and decreases operational costs [132]. The synthesis of nanoparticles using green nanotechnology approaches utilizes sustainable biodegradable materials and environmentally friendly methods [133,134]. Scientists use industrial waste and agricultural residues to create nanomaterials at low costs and achieve pollution reduction in their synthesis process [135]. Fe_3O_4 nanoparticles efficiently remove heavy metals but face high regeneration costs. Metal oxide nanocatalysts improve biofuel yields yet remain expensive. Green synthesis from agricultural waste reduces costs and supports circular economy goals. Unmodified iron oxides and biosynthesized nanoparticles offer eco-friendly, scalable options, though challenges persist yield and industrial feasibility.

5.3. Environmental fate and biodegradability

The complete environmental disposition and natural breakdown of nanomaterials depend on multiple elements. The physical properties of engineered nanomaterials (ENMs) influence how they react with environmental elements, which affects their movement through the environment [136]. The fate of nanomaterials relies on attributes such as size, shape, surface chemistry, and surface area [137]. Such environmental conditions lead to modifications of nanomaterials over time, which change their properties and corresponding effects [138-140]. Nanomaterials typically exhibit remarkable transformations in their destiny even after external factors alter their basic characteristics. Long-term property changes in nanomaterials become crucial for environmental impact assessments because silver nanoparticles convert into silver chloride coatings in sodium chloride medium, while zinc oxide nanoparticles quickly become Zn^{2+} sorption complexes. Silver nanoparticles transform into silver chloride in saline water, while zinc oxide dissolves into Zn^{2+} ions, raising environmental risks. Carbon nanotubes persist with poor biodegradability, and graphene oxide degrades under UV but remains stable in dark conditions. In contrast, biopolymer-based nanomaterials show partial biodegradation, offering safer, sustainable alternatives.

6. Recent Advances and Innovations

The continuous progress in nanomaterials science enables applications across multiple sectors, including environmental cleanup and energy storage, along with healthcare activities and modern manufacturing technologies. Several novel advancements exist within the nanomaterials field.

6.1. Functionalized and smart nanomaterials

Research on functionalized and smart nanomaterials has intensified in recent years because these materials exhibit special properties that enable multiple applications in biomedicine. The materials demonstrate specificity toward different stimuli, allowing them to become flexible solutions when applied for particular goals [141,142]. The exceptional mechanical properties and thermal conductivity of carbon nanomaterials, along with their electrical properties, optical effects, and chemical capacities, make carbon nanotubes, nanospheres and nanofibers promising candidates according to researchers [143]. Scientists face the problems with nanomaterials, including cytotoxicity, alongside poor photostability, insufficient cell targeting abilities, and limited cellular uptake. Research teams address these issues by adding various polymers, including hyaluronan (HA), to improve nanomaterials' biocompatibility and stability, as well as cell-specific targeting abilities [144-149].

6.2. Nano-bio hybrid systems

The combination of nanoparticles with biomolecular recognition and catalytic functions enables nano-bio hybrid systems to produce materials with unrecognized capabilities [150-152]. These systems are useful for device fabrication, as well as biosensing and nanostructure synthesis. Nanoparticles of both metal and semiconductor variations are employed as activators and labels for redox enzymes and biorecognition signals, respectively [153]. The impact of nanoparticles on biomolecules leads to different types of interactions between these two entities. The structural features of carbon nanomaterials, along with protein type, determine whether they will promote or hinder amyloid fibrillation formation [154]. Surface modification of nanoparticles using coatings with ethylene glycol serves as an effective method to improve their biological compatibility when addressing with nonspecific biomolecule–nanoparticle interactions [155,156].

6.3. Multi-functional nanocomposites

Nanocomposite materials with multiple functions bring together nanoparticle properties and different polymers to create materials that enhance mechanical strength, optical performance and electrical activity as well as biological functions. The combination of nanoparticles with various polymer matrices has become important in recent years because they serve multiple applications across biomedical fields, pharmaceutical sectors and materials science [157-159]. Polymer matrices incorporate metal-based nanoparticles, nanocarbons, and clay particles during the process of synthesizing multifunctional nanocomposites. The combination of gold and iron oxide nanoparticles allows for hybrid synthesis as functional materials suitable for theragnostic applications, gene transport systems, and biosensing needs. At the same time, atmospheric pressure microplasma synthesis enables *in situ* creation of metal nanoparticles within poly (vinyl alcohol) hydrogels that yield antibacterial nanocomposites. The addition of nanoparticles to polymer matrices creates unforeseen properties and functions as part of this combination. The incorporation of nanoparticles into gel-based materials has produced composites that exhibit antibacterial characteristics in addition to magnetic behavior and near-infrared sensitivity, as well as catalytic activity along with magnetism. The material properties of biopolymer-clay nanocomposites prove superior to traditional composites which helps address environmental issues [160-162].

6.4. AI and machine learning integration in nanomaterial design

Machine learning (ML) mostly allows the catalytic performance and prediction of chiral surface interactions using DFT, GNNs, and other models. Generative design, reinforcement learning, streamlined synthesis and Bayesian optimization, etc. which ensure eco-friendly, scalable nanomaterials for environmental remediation. These technologies to anticipate nanomaterial characteristics, streamline production synthesis, and speed up new material development [163-168]. AI and ML systems have extensively analyzed achiral nanomaterials, but researchers need to develop these methods for chiral nanomaterials because they represent an emerging prospect for scientists to create sustainable chiral materials with strong optical properties and selectivity control [169]. The process of AI /ML begins with data handling, where techniques such as NLP, data mining, and knowledge graphs curate and process experimental and simulation datasets. Surrogate models ANN and random forests to forecast material structures and accelerate costly computations. Optimization and evolutionary algorithms had to screen new nanomaterials and optimize synthesis. Finally, application domains focus on drug delivery, toxicity prediction, eco-safety, and nanocomposite performance, enabling sustainable innovations.

7. Real-World Application Challenges

7.1. Large-scale production

The large-scale production of sustainable nanomaterials remains a significant challenge because most laboratory synthesis methods are optimized for small-batch preparation using controlled conditions and specialized reagents. When these methods are scaled up, it becomes difficult to maintain uniform particle size

Table 4. Case studies of AI and ML integration in nanomaterial design

Case study	Application domain	AI/ML method used	Key outcome	Ref.
Nanoparticle toxicity prediction	Biomedical / Safety assessment	Random Forest, LightGBM, to interpret features affecting toxicity	Identified key nanoparticle features (size, surface charge, etc.) influencing cytotoxicity, enabling faster screening for safe-by-design nanomaterials	[170]
Predicting TiO_2 photocatalytic degradation rates for air contaminants	Environmental / Photocatalytic remediation	ANN, Gradient Boosting Regressor, XGBoost, and CatBoost with Bayesian optimization; molecular fingerprints to encode organic contaminants	Accurate prediction of degradation rate constants, reducing need for trial-and-error experiments	[171]
ML-guided design of metal oxide photoanodes (PEC water splitting)	Renewable energy / Photoelectrochemical water splitting	Machine learning-driven materials informatics: dopant & composition screening, optimization of band gaps and stability under visible light, performance optimization	Accelerated discovery of high-performance photoanodes; moved design toward predictive optimization that balances efficiency, stability, and cost	[172]

distribution, surface chemistry, and structural stability. The additional steps required for chemical or biological functionalization often involve high costs, energy inputs, or toxic solvents, which reduce the overall sustainability and commercial viability of these nanomaterials. Another barrier is the translation from proof-of-concept laboratory systems to industrial-scale reactors, where mass transfer limitations, aggregation, and fouling further compromise product quality. These factors collectively highlight the urgent need for scalable, low-cost, and eco-friendly production strategies that balance performance with environmental safety and economic feasibility [16].

7.2. Wastewater treatment

Most conventional treatment plants are designed around established processes such as precipitation, coagulation-flocculation, sedimentation, and ion exchange, which are cost-effective and well-regulated. In contrast, nanomaterial-based approaches often require specialized configurations, including membrane-assisted systems, fixed-bed adsorption columns, fluidized-bed reactors, or magnetic separation units to ensure efficient recovery and reuse of nanoparticles. Retrofitting these advanced systems into existing treatment facilities can be both technically challenging and economically prohibitive. While laboratory studies frequently report high adsorption or removal efficiencies in batch experiments, these results are rarely reproduced under continuous flow or fixed-bed reactor conditions, where hydrodynamic constraints, mass transfer limitations, and competitive interactions with coexisting ions significantly reduce efficiency. Real wastewater streams, which contain organic matter, fluctuating pH, and diverse contaminants, further exacerbate these challenges, causing nanoparticle aggregation or loss of active sites. Therefore, successful integration will require not only the development of more robust nanomaterials that can withstand complex wastewater matrices, but also the design of hybrid treatment technologies that can seamlessly couple nanomaterials with conventional methods to enhance overall system resilience and cost-effectiveness [173].

7.3. Regulatory and safety hurdles

Regulatory and safety hurdles represent one of the most pressing obstacles to the real-world application of nanomaterials for heavy metal remediation. While numerous laboratory studies highlight their high efficiency in controlled environments, the potential risks associated with nanoparticle toxicity, leaching of active components, and their long-term fate in ecosystems are still poorly characterized. Regulatory ambiguity also hinders the development of consistent guidelines for the safe production, handling, and disposal of nanomaterials in industrial applications. Furthermore, the potential for nanoparticle release during synthesis, use, or regeneration raises occupational health and safety concerns that must be addressed through stringent monitoring and protective standards. Without clear regulations, industries remain hesitant to adopt nanomaterial-based technologies, despite their promising performance in pollutant removal. Therefore, establishing robust, internationally harmonized frameworks for environmental risk assessment, toxicity testing, and life-cycle sustainability evaluation is crucial to bridging the gap between laboratory innovation and large-scale practical deployment [174].

7.4. Maintenance and operational issues

Maintenance and operational issues further restrict real-world application. Nanomaterials in wastewater systems face rapid fouling due to organic matter, biofilm growth, or competing ions, which block active sites and reduce adsorption efficiency. Agglomeration is another problem, as colloidal nanoparticles tend to cluster under variable pH or ionic strength, lowering surface area and performance. Regeneration protocols are often harsh; acid washes or high-temperature treatments degrade functional groups and shorten material lifespan. Finally, long-term performance and stability remain unresolved. Many nanomaterials exhibit >95% removal efficiencies in initial cycles but lose effectiveness after repeated regeneration due to structural damage, leaching of functional groups, or irreversible metal binding. Zero-valent iron nanoparticles, for example, are prone to agglomeration and surface passivation, which reduce long-term redox activity. Similarly, thiol-functionalized adsorbents suffer from oxidation of –SH groups, limiting recyclability. While polymer or silica coatings can prolong stability, most reports still lack multi-cycle or long-term field data, which is essential to evaluate true sustainability [175].

8. Future Perspectives

The environmental decontamination and heavy metal removal potential of nanomaterials require attention to multiple barriers that limit their sustainable implementation. The main issue regarding nanomaterials concerns their potential detrimental effects on both the environment and human health [176,177]. To achieve systematic risk evaluations and green chemistry compliance, researchers must investigate the unknown effects that these materials have on ecosystems and human health. Long-term performance, along with scalability, constitutes significant barriers for nanomaterial-based remediation approaches to function sustainably. Applications of numerous nanomaterials in real-world remediation demonstrate superb adsorption properties during laboratory analyses, but researchers still need to establish their full-scale effectiveness [178]. The practical use of nanomaterials requires solutions for aggregation problems, together with stability and mechanical strength issues. The prospects for heavy metal remediation using nanomaterials appear promising despite existing obstacles. Research is focusing on developing more sustainable and environmentally friendly nanomaterials, such as those derived from green biotechnology and utilizing microorganisms for nanoparticle synthesis [179]. There is also a growing interest in the recycling of toxic metal species as precursors in the synthesis of smart nanomaterials, promoting a circular economy approach [180]. Future research should focus on addressing the identified challenges, developing cost-effective and efficient nanomaterials, and exploring their large-scale applications [181]. More research is required to study how nanomaterials used in remediation processes affect the environment through transport and natural distribution patterns. The successful implementation of heavy metal removal and decontamination strategies depends on the ability to address operational obstacles and exploit nanomaterials' distinct characteristics. On the policy side, governments should establish strict regulatory frameworks, standardized testing protocols, and provide funding for pilot-scale demonstrations. Encouraging academia–industry partnerships will accelerate technology transfer, while circular economy strategies can promote nanomaterial reuse and recycling. Public awareness, training, and incentives are crucial to ensure safe, cost-effective, and widespread industrial adoption of sustainable nanotechnologies.

9. Conclusion

Heavy metal contamination creates a major environmental hazard that harms human health, necessitating the use of sustainable approaches to remediate contaminated sites. Nanotechnology excels in heavy metal remediation because these materials demonstrate superior capabilities through their vast surface area and customizable characteristics, which support multiple decontamination processes comprising adsorption and ion exchange, redox reactions, and chelation. The formation of sustainable nanomaterials through synthesis pathways that utilize biological plant elements combined with waste products addresses the resource scarcity problems and sustainability requirements. Long-lasting environmental effects, extensive production scale-up, and expense evaluations receive proper assessment despite the beneficial aspects of these materials. Life Cycle Assessment (LCA) provides valuable insights regarding nanomaterials by assessing significant features, including their ability to decompose naturally and material reuse capacity. Future research should focus on improving material synthesis techniques while enhancing material longevity and implementing safe guidelines for nanomaterial use. The combination of scientific innovation and environmental and economic priorities allows sustainable nanomaterials to serve as powerful agents for developing scalable heavy metal remediation solutions.

Acknowledgements

None.

Conflict of Interest

No conflicts of interest were reported by the authors in this work.

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