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Metal Coordination Complexes for Environmental Remediation: Recent Advances in Water Purification, Wastewater Treatment, and Pollution Control

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Abstract

Environmental pollution resulting from rapid industrialization, urbanization, agricultural intensification, and population growth has become one of the most pressing global challenges of the twenty-first century. Contamination of water resources by heavy metals, dyes, pharmaceuticals, pesticides, microplastics, endocrine-disrupting chemicals, and emerging organic pollutants poses serious threats to ecosystems and human health. Conventional treatment technologies often exhibit limited efficiency, high operational costs, poor selectivity, and secondary waste generation. Metal coordination complexes have recently emerged as highly promising functional materials for environmental remediation owing to their tunable molecular structures, high catalytic activity, excellent adsorption capacity, redox properties, and structural versatility. Coordination compounds incorporating transition metals and multifunctional organic ligands have demonstrated remarkable performance in photocatalysis, advanced oxidation processes, adsorption, membrane technologies, electrochemical treatment, and pollutant sensing. Furthermore, recent developments in metal-organic frameworks (MOFs), coordination polymers, nanocomposites, and green synthesis have significantly expanded their environmental applications. This review discusses the chemistry, synthesis, structural properties, remediation mechanisms, applications in water purification and wastewater treatment, recent technological advances, current challenges, and future prospects of metal coordination complexes in sustainable environmental management.

Keywords: *Metal coordination complexes, Environmental remediation, Water purification, Wastewater treatment, Heavy metal removal.*

1. Introduction

Water pollution has become one of the most critical environmental problems affecting public health, biodiversity, agricultural productivity, and sustainable economic development. Rapid industrial expansion, mining activities, pharmaceutical manufacturing, textile industries, petrochemical processing, agricultural runoff, and municipal wastewater discharge continuously introduce a wide variety of contaminants into aquatic ecosystems [1]. Heavy metals such as lead, mercury, cadmium, chromium, arsenic, and nickel, together with synthetic dyes, pesticides, pharmaceutical residues, endocrine-disrupting compounds, personal care products, antibiotics, microplastics, and persistent organic pollutants, exhibit long environmental persistence, bioaccumulation, and severe toxicity even at low concentrations. Consequently, the development of efficient, selective, economical, and environmentally sustainable remediation technologies has become an international research priority.

Conventional wastewater treatment methods, including coagulation-flocculation, chemical precipitation, activated sludge processes, membrane filtration, ion exchange, and activated carbon adsorption, have been widely applied for pollutant removal. However, these technologies often suffer from significant limitations such as incomplete contaminant removal, high energy consumption, sludge generation, poor selectivity toward emerging contaminants, membrane fouling, and expensive operational requirements. Increasingly stringent environmental regulations have therefore stimulated the search for advanced materials capable of addressing complex pollution challenges [2]. Metal coordination complexes have emerged as highly versatile materials for environmental remediation because their structural and electronic properties can be precisely tailored through careful selection of metal ions and coordinating ligands. Transition metals including iron, copper, cobalt, manganese, nickel, zinc, titanium, vanadium, cerium, and ruthenium readily form coordination compounds possessing catalytic activity, adsorption capability, redox functionality, and remarkable chemical stability. These complexes participate in pollutant degradation through photocatalysis, Fenton-like oxidation, electron transfer reactions, adsorption, ion exchange, and catalytic reduction processes. Recent advances in coordination chemistry have resulted in the development of highly porous metal-organic frameworks (MOFs), coordination polymers, supramolecular coordination assemblies, hybrid nanocomposites, and multifunctional catalysts with exceptionally large surface areas and tunable pore structures. Integration of coordination complexes with nanotechnology has further improved pollutant adsorption, catalytic efficiency, membrane performance, and environmental sensing [3]. Additionally, green synthesis approaches utilizing plant extracts, biodegradable ligands, and renewable materials have enhanced the sustainability of coordination-based remediation technologies. This review presents a comprehensive overview of recent advances in metal coordination complexes for environmental remediation, emphasizing their chemistry, synthesis, pollutant removal mechanisms, applications in water purification and wastewater treatment, technological innovations, challenges, and future research opportunities.

2. Chemistry and Structural Characteristics of Metal Coordination Complexes for Environmental Applications

Metal coordination complexes are molecular assemblies formed through coordinate covalent bonds between central metal ions and surrounding ligands containing electron-donating atoms such as oxygen, nitrogen, sulfur, or phosphorus. The remarkable versatility of coordination chemistry enables the rational design of materials with controlled geometry, porosity, electronic properties, catalytic activity, and chemical stability, making these complexes highly attractive for environmental remediation. Transition metal ions are particularly suitable for environmental applications because of their variable oxidation states and ability to participate in reversible redox reactions. Iron, copper, cobalt, manganese, nickel, titanium, zinc, cerium, vanadium, chromium, and ruthenium are among the most extensively investigated metals owing to their catalytic efficiency and environmental compatibility [4]. The choice of metal significantly influences pollutant degradation pathways, adsorption capacity, photocatalytic activity, and regeneration performance. Ligands play an equally important role by determining the stability, coordination geometry, pore architecture, and surface functionality of the resulting complexes. Organic ligands including carboxylates, amino acids, Schiff bases, porphyrins, phthalocyanines, bipyridines, phenanthrolines, imidazoles, terephthalic acid, and naturally derived polyphenols provide multiple coordination sites that stabilize metal centers while introducing functional groups capable of interacting with pollutants through hydrogen bonding, electrostatic attraction, π–π interactions, or coordination [5]. The coordination environment determines the geometry of the complex, which may adopt octahedral, tetrahedral, square planar, square pyramidal, trigonal bipyramidal, or polymeric structures. These geometries directly influence catalytic activity, electron transfer efficiency, adsorption selectivity, and photocatalytic performance. Metal-organic frameworks (MOFs) represent one of the most advanced classes of coordination materials, consisting of metal clusters interconnected by organic ligands to generate highly porous crystalline networks with exceptionally large surface areas exceeding several thousand square meters per gram. Recent developments have focused on hybrid coordination materials incorporating magnetic nanoparticles, graphene oxide, carbon nanotubes, biochar, activated carbon, cellulose, chitosan, and polymeric supports. These hybrid materials combine the advantages of coordination chemistry with improved mechanical strength, recyclability, adsorption efficiency, and environmental stability. The resulting multifunctional materials exhibit excellent potential for simultaneous removal of multiple contaminants from complex wastewater matrices.

Table 1: Common Metal Coordination Complexes Used in Environmental Remediation

Metal Ion	Common Ligands	Major Environmental Applications	Target Pollutants
Fe(III)/Fe(II)	EDTA, Carboxylates, Schiff bases	Fenton oxidation	Organic pollutants, dyes
Cu(II)	Bipyridine, Phenanthroline	Photocatalysis	Pharmaceuticals, dyes
Zn(II)	Imidazole, Carboxylates	Adsorption	Heavy metals
Ti(IV)	Organic acids	Photocatalysis	Organic contaminants
Co(II)	Schiff bases	Catalytic oxidation	Industrial wastewater
Mn(II)	Polyphenols	Advanced oxidation	Phenolic compounds
Ce(IV)	Organic ligands	Redox catalysis	Emerging contaminants

3. Mechanisms of Pollutant Removal by Metal Coordination Complexes

The exceptional efficiency of metal coordination complexes in environmental remediation arises from their ability to remove contaminants through multiple complementary mechanisms. Unlike conventional adsorbents that primarily rely on physical adsorption, coordination compounds combine adsorption, catalysis, oxidation, reduction, ion exchange, complexation, and photochemical degradation, thereby enabling simultaneous treatment of diverse classes of pollutants.

Adsorption remains one of the most important removal mechanisms. Functional groups present on coordination complexes interact with pollutants through electrostatic attraction, hydrogen bonding, π–π stacking, hydrophobic interactions, and coordination bonding [6]. Heavy metal ions are efficiently captured through chelation with oxygen-, nitrogen-, or sulfur-containing donor atoms, while organic contaminants are retained through surface adsorption and pore filling within porous coordination frameworks. Catalytic oxidation represents another highly effective remediation mechanism.

Transition metal complexes activate oxidizing agents such as hydrogen peroxide, ozone, and persulfates to generate highly reactive oxygen species, including hydroxyl radicals, sulfate radicals, and superoxide radicals. These reactive intermediates rapidly oxidize dyes, pharmaceuticals, pesticides, endocrine-disrupting chemicals, and persistent organic pollutants into smaller, less toxic molecules or complete mineralization products consisting of carbon dioxide and water.

Photocatalysis has become one of the fastest-growing applications of coordination complexes. Under ultraviolet or visible light irradiation, semiconductor-based coordination materials and metal-organic frameworks generate electron-hole pairs that initiate oxidative and reductive degradation reactions. Efficient charge separation within these materials minimizes electron-hole recombination and significantly enhances photocatalytic efficiency. Coordination complexes also participate in ion exchange and selective complexation processes for heavy metal removal [7]. Metal ions such as Pb^{2+}, Cd^{2+}, Hg^{2+}, As^{3+}, Cr^{6+}, and Ni^{2+} coordinate strongly with donor atoms present in the ligand framework, enabling selective removal even in complex wastewater containing multiple competing ions. Some coordination materials additionally exhibit magnetic properties, allowing simple recovery using external magnetic fields and facilitating repeated reuse without significant loss of activity.

The synergistic combination of adsorption, catalysis, photocatalysis, and redox chemistry enables coordination complexes to outperform many conventional treatment technologies in terms of efficiency, selectivity, regeneration, and operational sustainability.

Table 2: Major Pollutant Removal Mechanisms

Mechanism	Process	Primary Pollutants Removed
Adsorption	Surface binding	Heavy metals, dyes
Coordination/Chelation	Metal ion complexation	Pb^{2+}, Cd^{2+}, Hg^{2+}
Photocatalysis	Light-induced degradation	Pharmaceuticals, pesticides
Advanced Oxidation	Hydroxyl radical formation	Organic pollutants
Catalytic Reduction	Electron transfer	Hexavalent chromium
Ion Exchange	Replacement of ions	Heavy metals
Membrane Catalysis	Filtration and degradation	Mixed wastewater contaminants

4. Applications of Metal Coordination Complexes in Water Purification

The increasing contamination of freshwater resources has intensified the search for highly efficient treatment technologies capable of removing both conventional and emerging pollutants. Metal coordination complexes have attracted considerable attention because of their exceptional adsorption capacity, catalytic activity, chemical stability, and structural tunability. These materials have demonstrated outstanding performance in removing heavy metals, synthetic dyes, pharmaceutical residues, pesticides, endocrine-disrupting compounds, phenolic contaminants, and pathogenic microorganisms from drinking water and industrial effluents [8]. Heavy metal removal represents one of the most important environmental applications of coordination complexes. Toxic metals such as lead, cadmium, mercury, chromium, arsenic, copper, and nickel persist in aquatic environments and accumulate within living organisms, causing neurological disorders, kidney damage, carcinogenesis, and developmental abnormalities. Coordination complexes containing nitrogen-, oxygen-, and sulfur-rich ligands effectively chelate these toxic metal ions through stable coordination bonds. Porous metal-organic frameworks (MOFs), Schiff-base complexes, and functionalized coordination polymers exhibit exceptionally high adsorption capacities because of their abundant active sites and large specific surface areas. Synthetic dyes released from textile, leather, paper, printing, and food industries constitute another major category of water pollutants. Many dyes exhibit high chemical stability and resist conventional biological degradation. Metal coordination complexes efficiently remove these dyes through adsorption, photocatalytic oxidation, and advanced oxidation reactions. Under visible or ultraviolet irradiation, photocatalytic coordination materials generate reactive oxygen species capable of degrading dye molecules into smaller, less toxic compounds, thereby reducing color, chemical oxygen demand (COD), and total organic carbon (TOC). Pharmaceuticals and personal care products have recently emerged as contaminants of growing environmental concern because conventional wastewater treatment plants are often unable to eliminate them completely. Antibiotics, analgesics, hormones, antidepressants, and cosmetic ingredients enter aquatic environments through domestic sewage, hospitals, and pharmaceutical industries. Coordination complexes containing iron, titanium, copper, cobalt, and cerium exhibit remarkable catalytic efficiency for degrading these persistent organic compounds through photocatalysis, Fenton-like oxidation, and electrochemical oxidation [9]. Pathogenic microorganisms present in contaminated water also pose significant public health risks. Silver-, copper-, and zinc-based coordination complexes possess intrinsic antimicrobial activity by disrupting microbial membranes, generating reactive oxygen species, inhibiting essential enzymes, and damaging nucleic acids. These properties enable simultaneous water purification and disinfection, reducing dependence on conventional chlorination processes and minimizing the formation of harmful disinfection by-products. The incorporation of coordination complexes into filtration membranes, magnetic nanocomposites, activated carbon, graphene oxide, cellulose, and polymeric supports has further enhanced treatment efficiency by improving mechanical stability, regeneration capability, and continuous operation under practical conditions.

Table 3: Water Purification Applications of Metal Coordination Complexes

Water Contaminant	Representative Coordination Material	Removal Mechanism	Environmental Benefit
Lead (Pb^{2+})	Fe-MOFs	Chelation	Heavy metal removal
Cadmium (Cd^{2+})	Zn coordination polymers	Adsorption	Reduced toxicity
Chromium (Cr^{6+})	Fe-Schiff base complexes	Catalytic reduction	Detoxification
Textile dyes	Ti coordination complexes	Photocatalysis	Color removal
Antibiotics	Cu-MOFs	Advanced oxidation	Pharmaceutical degradation
Pesticides	Co coordination complexes	Catalytic oxidation	Organic pollutant degradation
Pathogenic bacteria	Ag coordination complexes	Antimicrobial action	Water disinfection

5. Metal Coordination Complexes in Wastewater Treatment and Pollution Control

Industrial and municipal wastewater contains highly complex mixtures of inorganic and organic contaminants that require integrated treatment strategies. Metal coordination complexes provide multifunctional remediation platforms capable of simultaneously removing multiple pollutant classes through adsorption, catalysis, oxidation, reduction, membrane separation, and ion exchange. Their versatility has expanded applications across textile, pharmaceutical, petrochemical, mining, food processing, electroplating, and agricultural wastewater treatment. Advanced oxidation processes (AOPs) employing metal coordination catalysts have become particularly effective for degrading refractory organic pollutants. Iron-, cobalt-, manganese-, and copper-based complexes activate oxidizing agents such as hydrogen peroxide, persulfate, peroxymonosulfate, and ozone to generate hydroxyl radicals and sulfate radicals. These highly reactive species rapidly mineralize persistent organic contaminants including pharmaceuticals, endocrine disruptors, phenols, chlorinated compounds, pesticides, and industrial solvents that resist biological degradation. Photocatalytic wastewater treatment has also experienced substantial growth with the development of visible-light-responsive coordination complexes. Metal-organic frameworks, porphyrin complexes, phthalocyanine derivatives, and hybrid photocatalysts efficiently harvest solar energy to produce reactive oxygen species capable of degrading organic pollutants without requiring excessive chemical additives [10]. This approach offers an environmentally sustainable alternative to conventional oxidation technologies [11]. Electrochemical treatment systems increasingly incorporate coordination complexes as electrocatalysts to improve oxidation efficiency while reducing energy consumption. These catalysts facilitate electron transfer reactions, accelerate degradation kinetics, and minimize electrode fouling during long-term operation. Simultaneously, membrane technologies modified with coordination complexes exhibit improved antifouling characteristics, selective permeability, antimicrobial activity, and catalytic degradation of membrane-retained pollutants. Air pollution control has likewise benefited from coordination chemistry. Certain coordination compounds efficiently adsorb volatile organic compounds (VOCs), sulfur dioxide, nitrogen oxides, and carbon dioxide, contributing to industrial emission control and greenhouse gas mitigation. Their tunable pore structures and high adsorption capacities enable selective capture of gaseous pollutants under diverse environmental conditions. The recyclability and regeneration of coordination complexes further enhance their economic feasibility. Many materials retain high catalytic and adsorption efficiency over multiple treatment cycles with minimal structural degradation, reducing operational costs and supporting sustainable wastewater management.

Table 4: Applications in Wastewater Treatment

Wastewater Source	Major Pollutants	Coordination Complex Application	Treatment Outcome
Textile industry	Synthetic dyes	Photocatalysis	Dye degradation
Pharmaceutical industry	Antibiotics, hormones	Advanced oxidation	Organic pollutant removal
Mining wastewater	Heavy metals	Adsorption and chelation	Metal recovery
Electroplating industry	Cr, Ni, Cu	Catalytic reduction	Metal detoxification
Municipal wastewater	Pharmaceuticals	MOF adsorption	Improved water quality
Agricultural runoff	Pesticides	Catalytic oxidation	Reduced toxicity

6. Recent Advances in Metal Coordination Complexes for Environmental Remediation

The field of coordination chemistry has advanced rapidly with the emergence of highly engineered materials designed specifically for environmental applications. Metal-organic frameworks (MOFs), coordination polymers, covalent-organic framework hybrids, nanocomposites, and magnetic coordination materials have significantly expanded the capabilities of traditional coordination complexes. These advanced materials exhibit exceptionally high surface areas, tunable pore architectures, superior catalytic efficiency, and excellent chemical stability. Among these developments, MOFs represent one of the most promising classes of environmental materials. Their crystalline porous structures provide abundant adsorption sites and facilitate rapid diffusion of pollutants throughout the framework. Functionalization of MOFs with amino, sulfonic acid, thiol, phosphonate, or carboxyl groups further enhances selectivity toward specific contaminants. Recent studies have demonstrated MOFs capable of simultaneously removing heavy metals, dyes, pharmaceuticals, pesticides, and radionuclides from contaminated water. Nanotechnology has substantially improved the performance of coordination complexes. Hybrid materials combining coordination compounds with graphene oxide, carbon nanotubes, activated carbon, biochar, magnetic iron oxide nanoparticles, cellulose nanofibers, and biodegradable polymers exhibit enhanced adsorption capacity, mechanical strength, electron transport, and recyclability. Magnetic nanocomposites are particularly attractive because they can be rapidly separated from treated water using external magnetic fields.

Artificial intelligence, machine learning, and computational chemistry have recently emerged as valuable tools for designing coordination complexes with optimized environmental performance. Molecular simulations, density functional theory calculations, quantitative structure–activity relationship (QSAR) modeling, and machine learning algorithms facilitate prediction of adsorption capacity, catalytic activity, stability, and pollutant selectivity before experimental synthesis [12]. These computational approaches significantly reduce development time and accelerate discovery of highly efficient remediation materials. Green chemistry has also become an important research direction. Bio-based ligands derived from amino acids, polysaccharides, lignin, tannins, flavonoids, and other renewable natural products are increasingly replacing synthetic ligands. Environmentally friendly synthesis methods minimize hazardous solvents and reduce energy consumption while maintaining high catalytic performance.

7. Challenges and Future Perspectives

Despite remarkable progress, several challenges continue to limit the widespread implementation of metal coordination complexes in environmental remediation. Large-scale production remains relatively expensive because of complex synthesis procedures, high-purity ligands, and sophisticated characterization requirements. Improving cost-effectiveness through simplified synthesis and renewable raw materials remains an important research priority. Long-term structural stability under diverse environmental conditions also requires further investigation. Changes in pH, ionic strength, temperature, competing ions, and natural organic matter may influence catalytic activity, adsorption efficiency, and framework integrity. In some cases, partial leaching of metal ions raises concerns regarding secondary environmental contamination, emphasizing the importance of developing highly stable and environmentally benign coordination materials. Regeneration and reuse are essential for practical wastewater treatment applications. Although many coordination complexes retain excellent performance after repeated cycles, gradual deactivation due to fouling, structural degradation, or active-site blockage remains a challenge. Future materials should combine high catalytic efficiency with simple regeneration procedures and long operational lifetimes. Future research is expected to focus on multifunctional coordination materials capable of simultaneously adsorbing, catalyzing, sensing, and degrading multiple pollutants. Integration with artificial intelligence, nanotechnology, membrane engineering, solar photocatalysis, electrochemical systems, and circular economy principles will likely produce highly efficient next-generation remediation technologies. Development of biodegradable ligands, low-cost synthesis strategies, renewable materials, and scalable manufacturing processes will further support commercialization and sustainable environmental management.

8. Conclusion

Metal coordination complexes have emerged as highly versatile and efficient materials for environmental remediation owing to their exceptional structural diversity, tunable coordination chemistry, catalytic activity, adsorption capacity, and redox properties. Through careful selection of metal ions and ligands, these materials can be engineered to remove a broad spectrum of environmental contaminants, including heavy metals, synthetic dyes, pharmaceuticals, pesticides, endocrine-disrupting compounds, pathogenic microorganisms, and other emerging pollutants from water and wastewater. Recent advances in coordination chemistry have led to the development of highly porous metal-organic frameworks, coordination polymers, hybrid nanocomposites, magnetic catalysts, and multifunctional photocatalysts that significantly outperform many conventional treatment technologies. Their ability to combine adsorption, photocatalysis, advanced oxidation, catalytic reduction, membrane separation, and pollutant sensing within a single material provides considerable advantages for sustainable pollution control. The integration of coordination complexes with green chemistry, nanotechnology, artificial intelligence, computational modeling, and renewable bio-based ligands has further accelerated innovation in environmental remediation. These developments have improved pollutant selectivity, catalytic efficiency, regeneration capability, and environmental compatibility while reducing energy consumption and secondary waste generation.

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