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Graphene/Carbon Nanocomposites for the Removal of Heavy Metal Ions from Water: A Research Progress Review

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ABSTRACT

Wastewater containing heavy metal ions produced during industrialization presents a significant danger to both the aquatic environment and human health. Developing efficient and economical heavy metal removal technologies has become a crucial research direction in environmental science. Graphene and carbon nanotubes, being representative carbon nanomaterials, exhibit distinctive structural characteristics, exceptionally high specific surface areas, and remarkable physicochemical properties, highlighting their significant potential for removing heavy metal ions from water. This paper systematically reviews the research progress of graphene/carbon nanocomposites in the field of heavy metal ion removal from water. It first elaborates on the functionalization strategies of such materials and analyzes the optimization effects of different modification methods on adsorption performance,selectivity, and recyclability. Secondly,it clarifies the core mechanisms by which the composites remove heavy metal ions, revealing the microscopic nature of the adsorption process through theoretical calculation methods. It also introduces the application and theoretical research findings of graphene- based membrane materials for heavy metal ion sieving and separation. Finally, it summarizes the key challenges currently facing the large-scale application of such materials and provides prospects for future research directions.

KEYWORDS

Graphene; Carbon nanotubes; Nanocomposites; Heavy metal ions; Wastewater treatment; Adsorption separation

1 Introduction

With the rapid development of global industrialization and manufacturing, the discharge of industrial wastewater containing heavy metal ions from industries such as metal plating, mining,and chemical manufacturing has continuously increased, significantly altering the hydrochemical characteristics of watershed ecosystems. Unlike organic pollutants, heavy metals such as lead (Pb^{2+}), copper (Cu^{2+}), cadmium (Cd^{2+}), and mercury (Hg^{2+}) cannot be biodegraded,exhibit clear biotoxicity even at extremely low concentrations,and can bioaccumulate through the food chain,causing long - term irreversible damage to ecosystem stability and human health, including kidney and nervous system damage, and even cancer.

Conventional heavy metal wastewater treatment technologies mainly include chemical precipitation, ion exchange, and conventional adsorption. While they can effectively remove some heavy metals,each method has notable limitations chemical precipitation produces large quantities of sludge containing heavy metals, leading to secondary pollution; ion exchange efficiency drops significantly when handling high - concentration wastewater, and the costs of material regeneration are high. Therefore, developing novel water purification materials and technologies with high adsorption capacity, high selectivity,and environmental friendliness has become a core research topic in the field of environmental engineering[1].

The swift advancement of nanotechnology presents significant opportunities for innovation in water treatment methods. Graphene and carbon nanotubes, which are representative carbon - based nanomaterials, feature unique structures—graphene is a two - dimensional honeycomb sheet, while carbon nanotubes are one - dimensional hollow tubes. They exhibit an exceptionally high specific surface area, remarkable chemical stability, and modifiability, demonstrating significant potential for applications in pollutant adsorption and membrane separation[2]. By utilizing functionalization design,specific functional groups can be added to the material ' s surface,or functional nanoparticles can be incorporated,thereby enhancing their adsorption selectivity, capacity,and recovery performance for heavy metal ions. Based on this, this paper systematically reviews the research progress of graphene/carbon nanocomposites in the removal of heavy metal ions from water, comprehensively elaborating on the functional design strategies, pollutant removal performance, mechanisms, and theoretical research findings of the materials, while analyzing current research challenges and future development directions, aiming to provide a theoretical reference for the practical application of such materials in water treatment[3].

2 Fundamental Properties of Carbon Nanomaterials

2.1 Structure and Properties of Carbon Nanotubes

Carbon nanotubes can be described as one - dimensional hollow tubular nanomaterials created by rolling up graphene sheets. They can be categorized into single - walled carbon nanotubes and multi - walled carbon nanotubes (

MWCNTs) based on the number of tube walls. This material features an extremely large aspect ratio,excellent mechanical strength and electrical conductivity, good chemical stability, and a considerable specific surface area, making it an ideal matrix material for preparing high - efficiency adsorbents[4]. However, pristine carbon nanotubes have inert surfaces, strong hydrophobicity, and strong van der Waals forces between tubes, leading to easy agglomeration in aqueous solutions and insufficient adsorption specificity for heavy metal ions, necessitating functionalization to optimize their application performance[5].

2.2 Structure and Properties of Graphene

Using sp hybridization, graphene is a two - dimensional atomic crystal made up of carbon atoms in a hexagonal honeycomb lattice. It has very high electron mobility,excellent thermal conductivity,and a theoretical specific surface area of approximately 2630 m^2/g. Its two-dimensional layered structure provides abundant reaction sites for surface functionalization modification, and nanofluidic channels can be constructed through interlayer structure regulation, making it an ideal building block for preparing high-performance adsorption composites and functional separation membranes[6]. Similar to carbon nanotubes, pristine graphene sheets are prone to stacking and agglomeration due to van der Waals forces and have poor dispersibility in water, requiring modification to overcome application bottlenecks[7].

3 Functionalization Methods of Graphene/Carbon Nanocomposites

The surface inertness and agglomeration issues of pristine carbon nanotubes and graphene limit their direct application in heavy metal ion removal. Surface functionalization is a fundamental way to improve their application performance, which is primarily separated into covalent functionalization and non - covalent functionalization techniques[5].

3.1 Covalent Functionalization

Covalent functionalization primarily introduces oxygen - containing functional groups such as carboxyl (- COOH), hydroxyl (- OH),and carbonyl (- C=O) onto the carbon material surface via strong acid oxidation (mixed acid treatment). This method significantly improves the dispersibility of the material in aqueous solutions and provides abundant reaction sites for subsequent organic molecule grafting, making it the most common modification method for carbon nanomaterials[5].

Related studies have successfully prepared aminated magnetic multi - walled carbon nanotubes (MMWCNT - NH_2) by reacting oxidized multi - walled carbon nanotubes with organic amines such as hexamethylenediamine, diethylenetriamine, and triethylenetetramine, significantly enhancing the material's adsorption performance for anionic dyes and heavy metal ions[5]. Simultaneously, loading Fe_3O_4 magnetic nanoparticles onto the material endows the composite with excellent magnetic separation performance, effectively solving the difficulty of recovering nano-adsorbents after use and avoiding secondary pollution[7].

3.2 Non-covalent Functionalization

In order to modify functional molecules like surfactants and polymers onto the surface of carbon materials, non - covalent functionalization primarily depends on intermolecular interactions such as the hydrophobic interactions, hydrophobic contacts, and electrostatic adsorption. This modification method does not destroy the intrinsic sp^2 conjugated structure of the carbon material,allowing optimizationof dispersibility and surface chemical properties while retaining the original excellent physicochemical properties[1].

For example, using the cationic surfactant cetyltrimethylammonium bromide (CTAB), negatively charged carbon nanotubes and MXene nanosheets can self-assemble into a three-dimensional composite via electrostatic and hydrophobic interactions, imparting a positive charge to the material surface and significantly enhancing its adsorption performance for anionic heavy metal pollutants[3]. Non-covalent functionalization offers mild reaction conditions and simple processes.making it an important approach for the multifunctional design of carbon nanomaterials[4].

4 Adsorption Performance and Mechanisms of Carbon Nanocomposites for Heavy Metal Ions

4.1 Main Factors Affecting Adsorption Performance

The adsorption behavior of functionalized carbon nanocomposites for heavy metal ions in water is mainly influenced by factors such as solution pH, temperature, ionic strength,adsorbent dosage,and initial pollutant concentration[5].

4.1.1 Solution pH

The most important element influencing the adsorption process is pH. It not only affects the surface charge state of the adsorbent but also affects the existing form of heavy metal ions in the aqueous solution. For the aminated adsorbent MMWCNT - NH_2, under acidic conditions, the surface amino groups are protonated and positively charged, exhibiting

strong electrostatic attraction for anionic Cr (VI) ($HCrO_4^-$ or CrO_4^{2-}),while electrostatically repelling positively charged metal ions. In contrast, under alkaline conditions, oxidized carbon nanotubes with carboxyl and hydroxyl groups are deprotonated and negatively charged, making them more suitable for adsorbing positively charged metal cations like Pb, Cu,and Cd[2]. Current research indicates that for the majority of heavy metal ions,the adsorption capacity tends to rise with increasing pH within the range of 4 to 8. This phenomenon is mainly attributed to the greater negative charge developing on the adsorbent ' s surface and the enhanced hydrolysis of the metal ions.

4.1.2 Temperature

The impact of temperature on the adsorption process can be quantitatively assessed using thermodynamic parameters (ΔG^0 , ΔH^0 , ΔS^0). Current research suggests that the adsorption of most heavy metal ions on carbon nanocomposites occurs as a spontaneous exothermic process ($\Delta H^0<0, \Delta G^0<0$), with lower temperatures being more conducive to the adsorption reaction. Nonetheless, some adsorption processes are endothermic,showing an increase in adsorption capacity with rising temperatures[1].

4.1.3 Other Influencing Factors

Coexisting ions in water (Na^+,Ca^{2+},Al^{3+}) compete with target heavy metal ions for adsorption sites, with higher valence ions exhibiting stronger competition, generally leading to decreased adsorption efficiency[5]. Increasing the dosage of the adsorbent can enhance the overall removal rate of heavy metal ions; however,it diminishes the unit adsorption capacity, as the excess adsorbent results in inadequate utilization of the surface active sites.

4.2 Core Mechanisms of Heavy Metal Ion Adsorption

The adsorption process of heavy metal ions from water by functionalized carbon nanocomposites results from the synergistic action of multiple mechanisms, with the core mechanisms mainly including the following categories[5,8].

4.2.1 Electrostatic Interaction

Electrostatic interaction is a key adsorption mechanism,in which surface functional groups on the adsorbent (such as protonated - NH_3^+ anddissociated - COO^-) directly attract and bind to oppositely charged heavy metal ions through electrostatic forces[5]. Zeta potential measurements are commonly used to characterize the variation of adsorbent surface charge with pH, thereby clarifying the core mechanism of pH influence on the adsorption process[8]. For example, the efficient removal of anionic Cr(VI) by positively charged MMWCNT-NH_2 is primarily driven by electrostatic attraction[5].

4.2.2 Surface Complexation / Coordination

Oxygen - containing functional groups (- COOH, - OH) and nitrogen - containing functional groups (- NH_2) on the surface of the material have lone pair electrons and can function as Lewis bases,forming coordination bonds with heavy metal ions that act as Lewis acids,thereby creating stable surface complexes[5]. This process is a type of chemisorption with high binding energy and is often irreversible. Among these, amino groups have a strong chelating ability for transition metal ions such as Cu and Pb,serving as a core pathway to boost the adsorption selectivity of the material[7].

4.2.3 Cation-π Interaction

Heavy metal ions can interact with the delocalized π electron clouds on the surface of graphene or carbon nanotubes via cation-π interactions, leading to adsorption and enrichment[8]. Density functional theory (DFT) calculations serve as essential instruments for investigating the characteristics and intensity of these interactions , shedding light on electron transfer and bonding between adsorbates and adsorbents at the atomic and molecular scale[6,8].

4.2.4 Other Mechanisms

Ion exchange is also an important adsorption mechanism. H^+ from surface functional groups or loaded cations such as Na^+ on the adsorbent can undergo ion exchange with heavy metal ions in the solution,achieving heavy metal removal[5]. Furthermore, the large specific surface area and porous structure of carbon nanomaterials can facilitate some physical adsorption through van der Waals forces; however,this is typically not the primary mechanism involved in the adsorption process.

4.3 Theoretical Calculation and Validation of Adsorption Mechanisms

Theoretical calculation methods play a vital role in clarifying the microscopic mechanisms of adsorption. Density functional theory (DFT) calculations can provide interaction energies, electron transfer, and bonding characteristics between adsorbate and adsorbent at the atomic/molecular level[6,8]. By calculating the adsorption energies of metal ions on carbon nanotubes modified with different functional groups, the promoting effect of different functional groups on adsorption performance can be quantitatively compared,and the donor-acceptor relationship of hydrogen bonds can be clarified[8]. The Independent Gradient Model utilizing Hirshfeld partitioning (IGMH) facilitates the visualization of weak interactions,such as van der Waals forces,hydrogen bonds,and steric hindrance,within the adsorption system.It allows for the direct identification of the regions and types of interactions,thereby offering an excellentmicroscopic explanation for experimental observations and theoretical support for the rational design of effective adsorbents.

Additionally, the Approximate Site Energy Distribution (ASED) theory is capable of examining the heterogeneity of the adsorbent surface from an energetic standpoint.Combining adsorption isotherm models with site energy distribution allows calculation of the number, distribution characteristics, and average site energy of different energy sites on the adsorbent surface,clarifying the preferential occurrence sites of the adsorption process and the effect of temperature on site energy heterogeneity, providing a novel analytical perspective for comparing adsorbent performance[8].

5 Application of Graphene - Based Membrane Materials in Heavy Metal Ion Separation

In addition to serving as adsorbents, graphene - based materials can also be utilized to create high - performance separation membranes that effectively reject heavy metal ions through a combination of physical sieving and electrostatic repulsion,marking a significant innovative research avenue in this area[3,6].

5.1 Graphene Oxide Nanofiltration Membranes

Graphene oxide (GO) membranes possess a unique structure of layered two-dimensional nanochannels, showing excellent application prospects in nanofiltration[6]. By adjusting the interlayer spacing and surface chemical properties of GO membranes,selective separation of ions and molecules of different sizes and charges can be achieved[3]. Studies have shown that for reduced graphene oxide (rGO) nanofiltration membranes prepared at different reduction temperatures, the water flux and dye rejection rate can be precisely controlled: the higher the reduction temperature,the fewer oxygen-containing functional groups on the material surface, the smaller the interlayer spacing,and although water flux slightly decreases, the rejection rate for the cationic dye methylene blue (MB) significantly increases due to enhanced electrostatic adsorption[6]. This separation mechanism based on charge effects is equally applicable to the separation of heavy metal ions with different charges[1].

5.2 Theoretical Study of Graphene Crown Pore Membranes

Molecular dynamics simulation is a fundamental tool for building atomically precise separation membranes. Related studies have constructed novel reverse osmosis membranes by designing "crown pores" with tunable shape and size on single-layer graphene, followed by protonation modification of the pore edges[8]. Simulation results show that the protonated crown pore graphene membrane achieves nearly 100% rejection of heavy metal ions such as Cd^{2+}, Cu^{2+}, Hg^{2+}, and Pb^{2+}, while maintaining high water flux[8]. The efficient rejection mechanism is primarily based on two factors first, the size sieving effect, where the hydrated radii of metal ions exceed the pore diameter, necessitating a significant energy barrier for partial dehydration to navigate through the pore;second, the electrostatic repulsion effect,where the positively charged hydrogen atoms at the protonated pore edges create a strong electrostatic repulsion with the positively charged heavy metal ions, thereby greatly hindering their transmembrane transport. This research provides important theoretical guidance for designing high-efficiency heavy metal ion separation membranes based on a charge-size dual screening mechanism[6,8].

6 Current Challenges and Future Prospects

6.1 Key Challenges for Large-Scale Application

Although graphene/carbon nanocomposites show excellent application prospects in the field of heavy metal pollution treatment, they still face many urgent problems in large-scale practical applications[1,4].

Firstly, there is the challenge of preparing materials on a large scale and managing costs effectively. Currently, the preparation processes for high-quality, structurally uniform graphene and carbon nanotubes are complex, making mass production difficult and costly, which is a core factor limiting their large-scale engineering application[4,7].

Second, the materials's long - term stability and cycling performance are insufficient. The anti-fouling and anti-corrosion performance of adsorbents in actual complex water environments directly determines their application value[5]. Although magnetic loading solves the material recovery problem, the adsorption performance of the material greatly deteriorates after multiple adsorption - desorption cycles, so improving the cycling life of the material is a critical current

research issue[7].

Third, unclear environmental fate and biosafety. The environmental behavior and potential ecological risks of carbon nanomaterials during and after use still lack systematic research[1]. According to recent research, certain carbon nanotubes have harmful effects on living things. Therefore, comprehensive evaluation of the environmental safety of the materials throughout their life cycle is needed, along with the development of green, environmentally friendly modification technologies and material systems[4].

Fourth, insufficient research on application in actual complex water bodies. The vast majority of current studies focus on single heavy metal pollutant systems, whereas actual industrial wastewater typically contains multiple heavy metal ions and coexisting organic pollutants[5]. Pollutants exhibit competitive adsorption and interference effects. The synergistic removal mechanisms and engineering application technologies for multi-component pollutants in complex systems still require in-depth research[1,3].

Fifth, challenges in the engineering implementation of graphene separation membranes. Graphene - based separation membranes experience inadequate structural stability during prolonged operation and under high - pressure conditions, while also encountering two significant challenges in the industry membrane fouling and the " trade - off " effect, which refers to the conflict between permeability and selectivity. These issues hinder their widespread adoption and application in real - world water treatment engineering.

6.2 Future Research Directions

Addressing the above issues, future research in this field can focus on the following directions: first, developing multifunctional integrated composites that combine adsorption, catalytic degradation, online monitoring, and other functions to expand application scenarios[1]; second, introducing artificial intelligence and machine learning technologies into material design to achieve accurate prediction and rational design of adsorbent and separation membrane performance[8]; third, deepening the combination of theoretical calculations and experimental research to systematically clarify interfacial interaction mechanisms in complex aquatic environments[6,8]; fourth, expanding the application of materials to environmental fields such as radionuclide removal and soil remediation to tap into the application potential of the materials[3-4].

7 Conclusion

Graphene and carbon nanotubes, with their unique structural features and excellent physicochemical properties, have clear application potential in the field of heavy metal ion pollution treatment[2,7]. Functionalizing the materials through covalent or non - covalent methods, such as introducing amino, carboxyl, or other functional groups and loading magnetic nanoparticles, can effectively boost the adsorption selectivity, capacity, and recyclability for target heavy metal ions[5,7]. The adsorption of heavy metal ions by the composites is driven by a combination of multiple mechanisms, such as electrostatic interactions, surface complexation, and cation - π interactions[5,8]. Meanwhile, theoretical calculation methods serve as essential tools for understanding the microscopic adsorption mechanisms[6,8]. Membrane separation technology based on graphene crown pore design offers a novel technical approach for efficient and energy-saving heavy metal ion rejection[8]. Although challenges remain in large-scale preparation, cost control, and environmental safety for these materials[1,4], with advances in material preparation technology and deepening fundamental research, graphene/ carbon nanocomposites will undoubtedly play an increasingly important role in water treatment and environmental protection[3].

References

[1] Yao, Y. Z., Hua, F., & Wu, K. (2024). Research progress of graphene-based composites for photocatalytic degradation of organic pollutants in wastewater. Industrial Water Treatment, 44(11), 1–8.

[2] Liu, J. L. (2025). Application of carbon nanotubes in water treatment. Papermaking Equipment & Materials, 54(9), 121–123.

[3] Lin, L., Li, L. F., & Li, J. H. (2025). New approach for seawater desalination and wastewater purification using multifunctional graphene composite hydrogels prepared by high-energy radiation irradiation technology. Journal of Radiation Research and Radiation Processing, 43(6), 06100.

[4] Wang, Z., Zhao, L., Ao, Q., et al. (2026). Research progress on preparation of biomass carbon nanotubes and application of related composites. Acta Materiae Compositae Sinica.

[5] Song, G. B. (2024). Study on adsorption mechanism of functionalized carbon nanotube composites for dyes in water [Doctoral dissertation]. Dalian Maritime University.

[6] Gao, Y. (2025). Study on the interaction at the graphene-water liquid-solid interface [Doctoral dissertation]. Kunming University of Science and Technology.

[7] Chu, R. (2025). Preparation and performance study of graphene/carbon nanotube composites. Shanxi Chemical Industry, (11), 54–56.

[8] Wang, S. T. (2025). Theoretical study on graphene crown pores for efficient removal of heavy metal ions [Doctoral dissertation]. Yangzhou University.