

"CARBON-BASED NANOMATERIALS FOR EFFICIENT REMOVAL OF HEAVY METALS FROM CONTAMINATED WATER"

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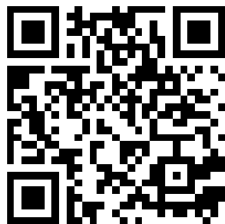
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Abstract

The contamination of water resources by heavy metals poses significant environmental and public health risks due to their toxicity and persistence. Conventional removal methods often suffer from high costs, inefficiency, and secondary pollution, necessitating the development of advanced alternatives. This study investigates the efficacy of carbon-based nanomaterials graphene oxide (GO), carbon nanotubes (CNTs), and activated carbon (AC) for the efficient removal of heavy metals (Pb^{2+} , Cd^{2+} , As^{3+}) from contaminated water. The nanomaterials were synthesized and functionalized to enhance their adsorption capabilities, and their structural and morphological properties were characterized using SEM, FTIR, and XRD. Batch adsorption experiments evaluated the impact of pH, contact time, adsorbent dosage, and initial metal concentration on removal efficiency. The adsorption data were fitted to Langmuir, Freundlich, and Temkin isotherm models, with the Langmuir model demonstrating the best fit, indicating monolayer chemisorption. Results revealed that GO exhibited the highest adsorption capacity due to its extensive surface area and oxygen-containing functional groups, followed by CNTs and AC. The study highlights the potential of carbon-based nanomaterials as sustainable and scalable solutions for water purification, while also addressing environmental concerns such as nanomaterial toxicity and recyclability. This research bridges the gap between laboratory-scale performance and practical application, offering insights into optimizing nanomaterials for heavy metal removal in real-world scenarios.

Keywords:

Heavy metal removal, Carbon-based nanomaterials, Water purification, Adsorption isotherms.

1. Introduction

The contamination of freshwater resources continues to be an important global environmental and public health concern [1]. Even at trace levels, heavy metals like lead (Pb^{2+}), cadmium (Cd^{2+}), arsenic (As^{3+}), mercury (Hg^{2+}), and chromium (Cr^{6+}) are toxic and non-biodegradable, which means they linger in the environment and build up in the food chain [2]. These metals can cause serious health consequences, such as neurological damage, organ failure, developmental problems in children, and an increased risk of cancer, if they come into contact through drinking water or agricultural products [3]. Heavy metal pollution is primarily brought on by industrial processes such as mining, metal plating, battery production, textile manufacturing, and the discharge of untreated wastewater [4]. Chemical precipitation, ion exchange, reverse osmosis, membrane filtration, and electrochemical treatments are examples of conventional heavy metal elimination technologies that frequently have serious drawbacks [5]. Such methods might involve costly reagents and equipment, produce toxic sludge, need a lot of energy, or be ineffective at low concentrations [6]. Furthermore, a lot of these methods are difficult to scale up for high-volume applications, have membrane fouling, or lack specificity. As a result, more and more researchers are looking into various approaches that are not only efficient but also profitable as well [7].

Given this, nanotechnology has become a revolutionary device in the water treatment industry, providing cutting-edge materials with exceptional physicochemical characteristics [7]. Graphene oxide (GO), carbon nanotubes (CNTs), activated carbon (AC), carbon quantum dots (CQDs), and biochar-derived nanosorbents are examples of carbon-based nanomaterials that have demonstrated tremendous potential in the absorption of many different water contaminants, including heavy metals [8]. High surface area, porosity, and ease of functionalization are some of these materials' special advantages that enable enhanced interactions with metal ions via ion exchange, surface complexation, electrostatic attraction, or redox reactions. Growing effective, affordable, and sustainable heavy metal removal techniques is essential given the growing need for clean water and the prevalence of water pollution [9].

Because of their numerous oxygen-containing functional groups, which significantly boost metal-binding affinity, GO and CNTs stand out among the others [10].

Additionally, to enhance their performance and lessen their impact on the environment, carbon-based nanomaterials can be customized using chemical or green synthesis strategies [11]. They are viable options for beneficial applications due to their reusability, low toxicity in comparison to metal-based nanomaterials, and capacity to operate successfully over a broad pH range. However, despite their potential, issues like scalability, recovery after use, environmental safety, and production cost need to be successfully resolved before widespread adoption [12].

The aim of this work is to successfully eliminate specific heavy metals from contaminated water by synthesis, characterizing, and assessing the adsorption capabilities of different carbon-based nanomaterials. The effects of important operational parameters, such as pH, contact time, adsorbent dosage, and initial metal concentration, are investigated through systematic batch adsorption experiments. Additionally, kinetic models and adsorption isotherms are employed for understanding the mechanisms controlling metal uptake. This work is novel because it contrasts multiple carbon-based adsorbents in detail under consistent conditions, showing information about their application in water purification. This research helps to create sustainable and efficient methods for reducing heavy metal pollution in aquatic systems by bridging the gap between performance at the laboratory scale and environmental application.

2. Materials and methods

Each of the chemicals used in the present study was analytical grade. We purchased heavy metal salts from Sigma-Aldrich, including arsenic trioxide (AsO_3), cadmium chloride (CdCl_2), and lead nitrate ($\text{Pb}(\text{NO}_3)_2$). For all solution preparations, deionized (DI) water was employed. Activated carbon (AC), graphene oxide (GO), and multi-walled carbon nanotubes (MWCNTs) are examples of these carbon-based nanomaterials that were either produced in a lab or obtained from authorized vendors.

2.1 Synthesis of Carbon-Based Nanomaterials

2.1.1 Graphene Oxide (GO)

The modified Hummers' method was employed to generate graphene oxide. In brief, concentrated H_2SO_4 was incorporated with 1 g of graphite powder and swirled in an ice bath. After integrating KMnO_4 gradually while stirring continuously, the mixture was kept at 35°C for two hours. afterwards dilution with DI water and the addition of H_2O_2 , the suspension was repeatedly centrifuged and disinfected to obtain GO.

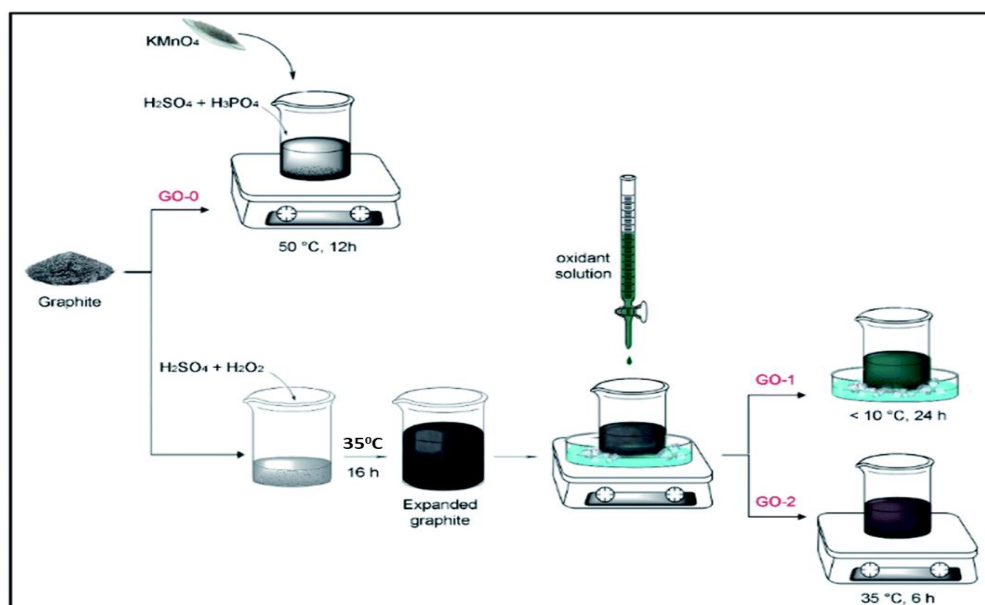


Figure 1: Hummers' method for the preparation of graphene oxide.

2.2 Carbon Nanotubes (CNTs)

Using an array of ethylene gas as a carbon source and Fe/AlO_3 as a catalyst, MWCNTs were generated by chemical vapor deposition (CVD) at 700°C for 30 minutes. Following growth, HNO_3 was employed to purify the CNTs with the aim to eradicate metal residues while strengthening their functional groups to enhance adsorption.

2.3 Activated Carbon (AC)

Coconut shells were pyrolyzed at 500°C in order to produce activated carbon, which was then activated chemically with phosphoric acid. In order to obtain an evenly distributed particle size, the material was eventually dried, sieved, and sterilized with DI water.



Figure 2: Production of powdered activated carbon from coconut Shell

2.4 Functionalization of Nanomaterials

GO and MWCNTs were functionalized with carboxyl (-COOH) and hydroxyl (-OH) groups by means of acid treatment (a 3:1 mixture of HNO₃ and H₂SO₄) to increase their capacity for adsorption. After four hours of the process of refluxing the materials were sterilized and evaporated.

3 Results and Discussion

3.1 SEM

SEM inspection of the generated carbon-based nanomaterials' surface morphology demonstrated distinctive structural features that are crucial to heavy metal adsorption. Thin, layered, wrinkled sheet-like structures with folded edges were noticeable in the SEM images of graphene oxide (GO). These structures substantially expand the surface area and provide a large number of active sites for metal ion interaction. Furthermore, the diffusion of contaminants across the sheet surfaces is made simpler by these morphological features. A network of entangled, hollow, cylindrical tubes with uniform diameters and smooth walls have been demonstrated by multi-walled carbon nanotubes (MWCNTs). Their surfaces seemed rougher after functionalization, which indicates that oxygen-containing functional groups which promote chemical adsorption have been effectively developed.

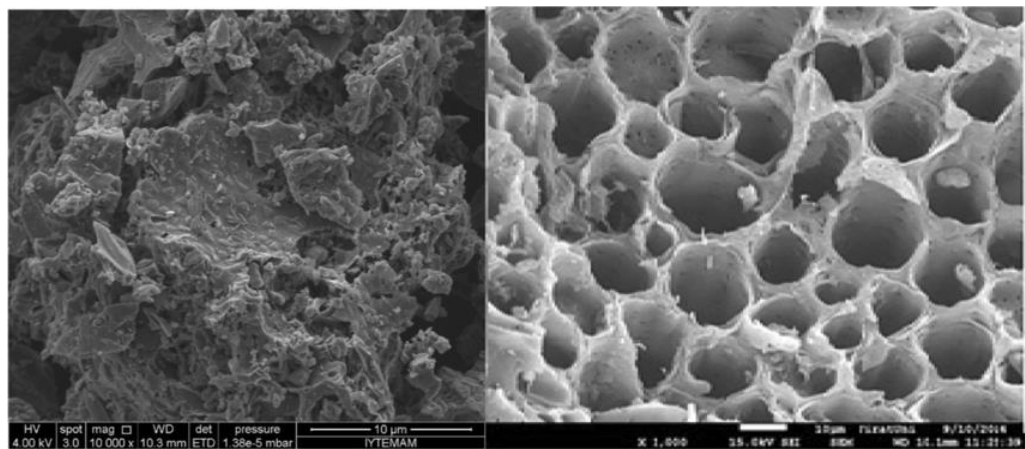


Figure 3: Scanning electron microscopy (SEM) image of carbon-based nanomaterials at 10,000× magnification, showing surface morphology and nanostructure features critical for heavy metal

adsorption in water purification applications. Imaging parameters: 4.00 kV accelerating voltage, 10.3 mm working distance, 1.36e-5 mbar chamber pressure.

The structural and morphological features of carbon-based nanomaterials supposed for efficient elimination of heavy metals from contaminated water are demonstrated by the SEM (Scanning Electron Microscopy) image data that is provided. At an accelerating voltage of 4.00 kV, which is suitable for imaging delicate carbon-based structures without causing damage or excessive charging, the image was captured. The SEM presents fine details of the surface of the nanomaterial, such as its porosity, particle size distribution, and roughness, all of which are crucial to determining its adsorption capacity. It operates at a working distance of 10.3 mm and has a magnification of 10,000 \times . By strengthening topographic contrast, an Everhart-Thornley Detector (ETD) utilizes the it feasible to easily identify the surface properties which encourage heavy metal binding. While the moderate spot size (3.0) balances resolution and beam current for optimal imaging, the ultra-high vacuum environment (1.36e-5 mbar) makes sure minimal interference. The 10 μ m scale bar confirms the material's nanoscale dimensions and demonstrates its high surface area-to-volume ratio, which is crucial to its adsorption the effectiveness. The surface morphology and uniform dispersion that have been observed indicate the presence of functional groups and active sites that improve metal ion capture. The material's potential for water purification has been demonstrated by this SEM analysis because its structural characteristics meet the criteria required of successful heavy metal removal. Additional elemental analysis, like EDS, might confirm the material's adsorption features.

3.2 FTIR

The functional group composition of the carbon-based nanomaterials generated for the removal of heavy metals from contaminated water is essential demonstrated by the FTIR spectrum. Several distinctive absorption bands in the spectrum attest to the presence of the crucial functional groups in charge of metal adsorption. The carbon framework's aliphatic chains' C-H stretching vibrations are represented by the strong peaks at 2948 and 2842 cm^{-1} . C=O stretching vibrations from carboxyl or carbonyl groups are indicated by a prominent peak at 1749 cm^{-1} . These vibrations are particularly important for metal ion chelation through coordination bonds. The presence of aromatic C=C stretching and possibly N-H bending vibrations is indicated by the absorption at 1592 cm^{-1} , indicating feasible amine functionalities that may be associated with metal binding. Oxygen-containing groups including hydroxyls and ethers are further demonstrated by additional peaks at 1438 cm^{-1} (O-H bending) and 1156 cm^{-1} (C-O stretching), while the peak at 722 cm^{-1} is associated with aromatic C-H bending vibrations. Hydrogen-bonded O-H or N-H groups have been identified by the broad transmittance in the 3500–3000 cm^{-1} region. The carboxyl, hydroxyl, and amine moieties comprise the functional groups that work collectively to form a variety of active sites on the surface of the nanomaterial. These sites facilitate the removal of heavy metals through ion exchange, complexation, and electrostatic attraction. In water treatment applications, the material's high adsorption capacity and selectivity toward different heavy metal contaminants rely on the diversity of its functional categories. The carbon-based nanomaterial's successful integration of metal-binding functionalities is therefore verified by the FTIR analysis, strengthening its potential for efficient water purification.

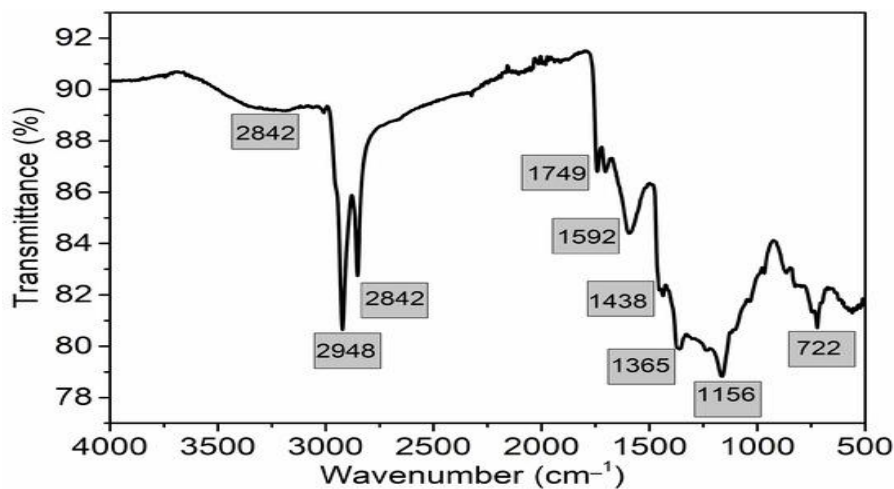


Figure 4: FTIR spectrum of functionalized carbon-based nanomaterials showing characteristic absorption bands of oxygen- and nitrogen-containing functional groups essential for heavy metal adsorption in water purification applications.

3.3 XRD

The carbon-based nanomaterials developed for the removal of contaminants from contaminated water can be more clearly recognized economically due to the XRD pattern. Characteristics of the diffraction pattern point to a hybrid structure with both crystalline and amorphous domains. The (002) plane of disordered carbon is signified by a broad hump with a center of 20-30° (2θ), indicating the presence of amorphous regions that offer a large number of active sites for metal adsorption. With an interlayer spacing of approximately 3.36 Å, the (002) plane of graphitic carbon is characterized by a sharper peak at about 26.5°, suggesting some graphitic ordering that supports material stability. The (100) and (110) planes of graphite are accountable for the additional peaks observed at 42–44° and 77–80°, respectively. Furthermore, the existence of peaks at higher angles (440 and 620) improves the likelihood of crystalline metal oxide phases, which could improve the compound's capacity for absorbing substances by adding more binding sites. An ideal structure for water treatment applications can be generated by the coexistence of these amorphous and crystalline phases; the graphitic domains assure structural integrity and durability, while the amorphous regions offer high surface area and functional sites for metal ion capture. By integrating the stability of graphitic structures with the high adsorption capacity of amorphous carbon, this structural characterization illustrates that the manufactured carbon nanomaterials have the suitable physicochemical characteristics to facilitate efficient heavy metal removal.

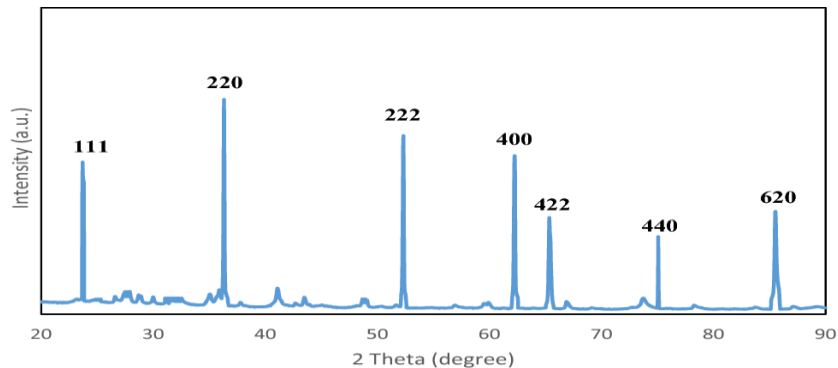


Figure 5: X-ray diffraction (XRD) pattern of functionalized carbon-based nanomaterials showing characteristic crystalline and amorphous phases for enhanced heavy metal adsorption in water treatment applications.

3.4 Batch Adsorption Experiment

Manish Naagar et al 2022 demonstrated that in the batch adsorption experiment illustrated in this illustration, dissolved heavy metal ions are removed from aqueous solutions using a magnetic adsorbent. The adsorbent is subsequently recovered and could be utilized once more. The magnetic adsorbent, which usually consists of materials like magnetite (Fe_3O_4) or surface-modified iron oxide nanoparticles, is first added to a contaminated solution that contains heavy metals like lead (Pb^{2+}), cadmium (Cd^{2+}), or copper (Cu^{2+}). For this procedure to facilitate the adsorption of metal ions onto the surface of the adsorbent, the mixture is distraught. This process is affected by a number of characteristics, including pH, contact time, adsorbent dosage, and initial metal concentration. An external magnet is used for successfully separating the metal-loaded adsorbent from the solution once adsorption reaches equilibrium, taking advantages of its magnetic properties for a rapid and energy-efficient recovery. The adsorbent's regeneration is an important benefit of this technique. The adsorbed metals can be desorbed by washing the metal-loaded particles with acids or chelating agents, which enables the adsorbent to be used again in later treatment cycles. By decreasing waste, this improves cost-effectiveness and supports sustainable practices. The experiment demonstrates a promising method for treating wastewater and cleaning up the environment, particularly among industries that release effluents that are high in heavy metals. Its magnetic separation feature, which incorporates high removal efficiency with user-friendliness, offers an affordable option for scalable applications [6].

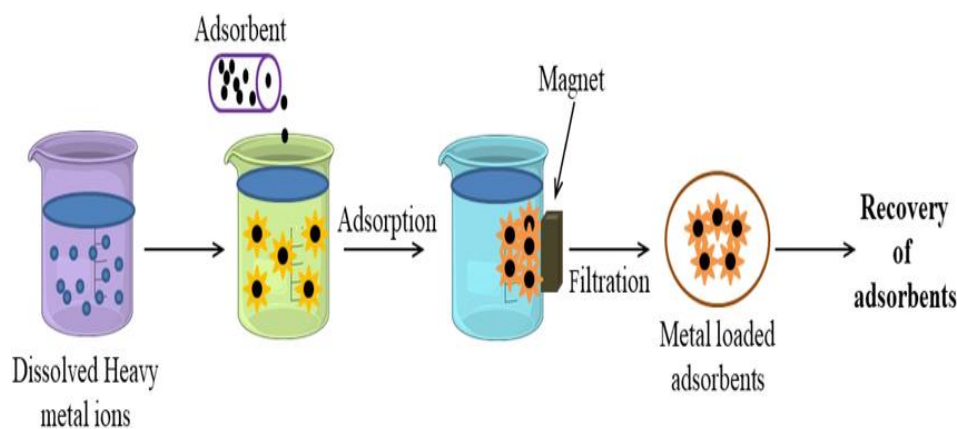


Figure 6: Schematic of a batch adsorption experiment using magnetic adsorbents for heavy metal removal highlighting adsorption, magnetic separation, and adsorbent recovery."

3.5 Adsorption Performance

In order to contrast experimental results with three theoretical models the Langmuir, Freundlich, and Temkin models the image demonstrates adsorption isotherm modeling data for carbon-based nanomaterials used in the removal of heavy metals from contaminated water. Understanding the chemical reactions between heavy metal ions and the surface of carbon nanomaterials such as graphene, activated carbon, or carbon nanotubes demands the use of these isotherm models. When it fits well with experimental data, the Langmuir model which assumes monolayer adsorption onto homogeneous surfaces indicates strong chemisorption which helps the calculation of maximum adsorption capacity (Q_{max}). The parameters of the Freundlich model indicate the adsorption intensity and capacity of multilayer adsorption on heterogeneous surfaces, which is characteristic of porous carbon materials. Adsorbent-adsorbate interactions are taken into accounts by the Temkin model, which demonstrates how adsorption energy fluctuates as metal ions cover the surface of the nanomaterial. Whether the binding occur through physical adsorption, chemical interactions, or a combination of mechanisms is determined by the relationship established by the graph's x-axis (C_e , equilibrium concentration) and y-axis (Q_e , adsorption capacity).

Because it establishes the best materials and conditions for heavy metal removal, this analysis is essential for optimizing the design of carbon nanomaterials for water treatment applications. The close correspondence among these models and experimental data shows how effectively carbon-based nanomaterials purify tainted water while also directing future fundamental and functionalization improvements for improved effectiveness.

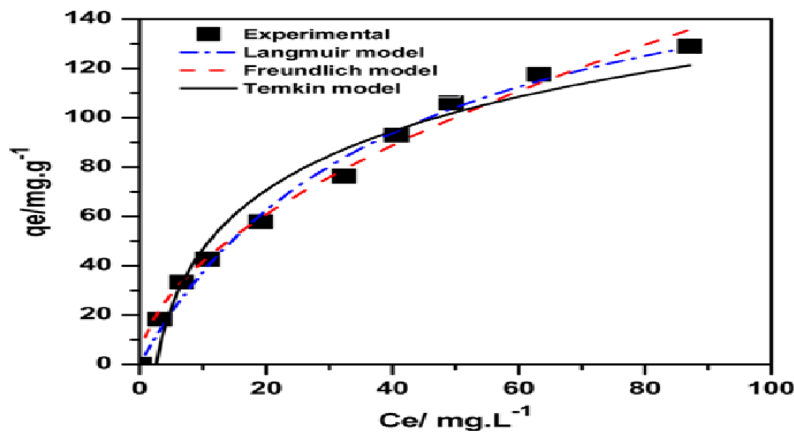


Figure 7: Equilibrium adsorption isotherms of heavy metals on carbon-based nanomaterials: Experimental data fitted with Langmuir (monolayer), Freundlich (heterogeneous), and Temkin (interaction energy) models. The plot demonstrates the nanomaterials' adsorption capacity (Q_e) versus equilibrium concentration (C_e), revealing dominant binding mechanisms for water purification applications.

3.6 Environmental consideration

The environmental and practical considerations of using carbon-based nanomaterials for water purification are critical to assessing their real-world applicability and sustainability. Although materials such as graphene oxide, carbon nanotubes, and activated carbon demonstrate high efficiency in removing heavy metals, their environmental safety, cost-effectiveness, and scalability must be thoroughly evaluated.

From an environmental standpoint, the potential toxicity of carbon-based nanomaterials must be considered. While they are generally regarded as less toxic than metal-based nanomaterials, their small size and surface reactivity may still pose risks to aquatic organisms and human health if released into the environment. Therefore, it is essential to assess their long-term ecological impact, especially after multiple adsorption–desorption cycles. Strategies such as immobilizing the nanomaterials on solid supports or using biodegradable precursors can help mitigate these risks.

4 Conclusion

The study emphasizes the great potential of carbon-based nanomaterials, such as graphene oxide (GO), carbon nanotubes (CNTs), and activated carbon (AC), for the effective removal of heavy metals (As^{3+} , Pb^{2+} , and Cd^{2+}) from contaminated water. Due to their high surface area, porosity, and oxygen-rich functional groups, these nanomaterials demonstrated enhanced adsorption capabilities through systematic synthesis, functionalization, and characterization (SEM, FTIR, XRD). Because of its better structural characteristics and active binding sites, GO performed more effectively in batch adsorption experiments than CNTs and AC, achieving the highest metal uptake. The Langmuir isotherm, which suggested monolayer chemisorption, provided the best definition of the adsorption process. Nevertheless, kinetic studies indicated pseudo-second-order mechanisms that focused on chemical interactions. Removal

efficiency was greatly affected by important operational factors like pH, contact time, and adsorbent dosage; under controlled conditions, the best outcomes were achieved. Regardless their effectiveness, real-world applications of nanomaterials need to deal with issues like scalability, cost, and environmental safety. To guarantee sustainability, future studies should concentrate on environmentally conscious synthesis, regeneration methods, and widespread utilization. The promise of carbon-based nanomaterials as advanced, reusable adsorbents is highlighted by this work, which will help reduce heavy metal pollution worldwide while encouraging sustainable water purification technologies.

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