



Invasive Biomass to Functional Nanoadsorbent: Parthenium hysterophorus-derived Magnetic Nanoparticles for Efficient Removal of Imidacloprid from Aqueous Systems

M. K. Muniyasamy^{1*}, D. Arivukkarasu², R. M. Saravanakumar³, Balkis Banu W⁴, Aravindan A⁵ and K. M. Basanth Babu⁶

¹Department of Civil Engineering, Saveetha Institute of Medical and Technical Sciences, Chennai, TN, India

²Department of Civil Engineering, GRT Institute of Engineering and Technology, Tiruttani, TN, India

³Department of Civil Engineering, Vel Tech Rangarajan Dr. Sagunthala R and D Institute of Science and Technology, Chennai, TN, India

⁴Department of Civil Engineering, Rajalakshmi Engineering College, Thandalam, Chennai, TN, India

⁵Department of Civil Engineering, Koneru Lakshmaiah Educational Foundation, Guntur, AP, India

⁶Department of Civil Engineering, Ultra College of Engineering and Technology, Madurai, TN, India

Received: 08.06.2026 Accepted: 15.06.2026 Published: 30.06.2026

*munishcivilian1@gmail.com



ABSTRACT

This study presents a sustainable approach for the synthesis of magnetic nano-adsorbents derived from the invasive plant *Parthenium hysterophorus* for the efficient removal of the pesticide imidacloprid from aqueous systems. A green co-precipitation method was employed using plant extract as a reducing and stabilizing agent to fabricate bio-functionalized Fe₃O₄ nanoparticles. Comprehensive characterization confirmed the successful formation of crystalline, superparamagnetic nanoparticles with enhanced surface functionality. The presence of phytochemical-derived functional groups significantly improved adsorption performance compared to chemically synthesized counterparts. Batch adsorption studies revealed that the removal efficiency was strongly influenced by pH, contact time, and adsorbent dosage, with optimal performance observed under near-neutral conditions. The green synthesized nanoparticles exhibited a maximum adsorption capacity of 105 mg/g and a surface area of 82.3 m²/g, significantly outperforming chemically synthesized counterparts. The adsorption process followed pseudo-second-order kinetics ($R^2 > 0.99$) and Langmuir isotherm behavior. Reusability studies showed retention of 68% efficiency after five cycles, confirming good stability. Catalytic degradation studies revealed 76% degradation efficiency within 90 minutes with a rate constant (k) of 0.018 min⁻¹, confirming the synergistic adsorption–degradation capability of the synthesized nanomaterial.

Keywords: Green synthesis; Magnetic nanoparticles; *Parthenium hysterophorus*; Imidacloprid removal; Water remediation.

1. INTRODUCTION

The rapid intensification of agricultural practices to meet the increasing food demands of a growing global population has led to the extensive use of synthetic pesticides, among which neonicotinoid compounds have gained significant prominence due to their high efficacy and systemic action (Kulkarni, 2023; Kundoo *et al.* 2018). One of the most widely used representatives of this class is Imidacloprid, which is extensively applied for the control of sucking insects in crops such as rice, cotton, and vegetables. Despite its agronomic benefits, the persistent and mobile nature of imidacloprid has raised serious environmental concerns, particularly due to its frequent detection in surface water, groundwater, and soil systems (Casillas *et al.* 2022; Bonmatin *et al.* 2015). Its high solubility in water and relatively long half-life contribute to its widespread distribution in aquatic environments, thereby posing

potential risks to non-target organisms, including pollinators, aquatic fauna, and even humans through bioaccumulation and trophic transfer (Zhang *et al.* 2022; Roodt *et al.* 2023; Lima-Fernandes *et al.* 2019).

Conventional wastewater treatment technologies, including biological degradation, coagulation–flocculation, and membrane filtration, have shown limited efficiency in the removal of such recalcitrant organic contaminants (Barco-Bonilla *et al.* 2010; Pang *et al.* 2020). This limitation is primarily attributed to the complex molecular structure and resistance of imidacloprid to biodegradation under typical environmental conditions. Moreover, advanced treatment processes such as ozonation and photocatalysis, although effective, are often associated with high operational costs, energy requirements, and the potential formation of toxic intermediate by-products (Bello and Raman, 2019; Kudlek, 2019).

In recent years, adsorption-based techniques have emerged as one of the most promising approaches for water purification due to their simplicity, high efficiency, and adaptability (Badran *et al.* 2023). Particularly, the use of nanomaterials as adsorbents has attracted considerable attention owing to their high surface area, tunable surface properties, and enhanced reactivity (Borthakur, 2025). Among these, magnetic nanoparticles, especially iron oxide (Fe_3O_4)-based materials, have been widely explored due to their unique advantage of easy separation from treated water using an external magnetic field, thereby eliminating the need for complex filtration or centrifugation processes (You *et al.* 2021; Simeonidis *et al.* 2011). However, conventional synthesis routes for magnetic nanoparticles often involve toxic chemicals and harsh reaction conditions, which contradict the principles of green chemistry and limit their large-scale applicability (Osman *et al.* 2024).

To address these challenges, the green synthesis of nanomaterials using plant-derived biomolecules has gained significant momentum as a sustainable alternative. Plant extracts are rich in bioactive compounds such as phenolics, flavonoids, alkaloids, and terpenoids, which can act as natural reducing, stabilizing, and capping agents during nanoparticle synthesis (Munir *et al.* 2021; Yousaf and Saleh, 2018). This approach not only minimizes the use of hazardous chemicals but also introduces functional groups on the nanoparticle surface, thereby enhancing their adsorption capacity and interaction with target pollutants (Das *et al.* 2023). In this context, the utilization of invasive plant species as biomass precursors offers a dual advantage of environmental remediation and ecological management.

One such highly invasive and problematic weed is *Parthenium hysterophorus*, commonly known as congress grass. It is widely distributed across India and poses severe threats to agriculture, biodiversity, and human health due to its allelopathic effects and allergenic properties (Kohli *et al.* 2006; Tefera, 2002). The uncontrolled proliferation of *Parthenium* has led to significant economic losses and ecological imbalance in several regions. Interestingly, this plant is rich in various phytochemicals, including sesquiterpene lactones, phenolic acids, and flavonoids, which can be effectively utilized for the green synthesis of nanomaterials (Ahsan *et al.* 2020). The valorization of such invasive biomass into functional nanoadsorbents represents a sustainable and innovative approach aligned with the concept of waste-to-wealth conversion.

Magnetic nanoparticles synthesized using *Parthenium* extract are expected to exhibit enhanced adsorption performance due to the synergistic effect of magnetic properties and bio-functionalized surfaces. The presence of oxygen-containing functional groups,

such as hydroxyl and carboxyl groups, facilitates strong interactions with pesticide molecules through mechanisms such as hydrogen bonding, electrostatic attraction, and π - π interactions (Masoudi *et al.* 2018; Law, 2008). Furthermore, these nanoparticles can potentially act as catalysts in advanced oxidation processes, enabling the degradation of imidacloprid into less harmful intermediates (Shahwan *et al.* 2011). The integration of adsorption and catalytic functionalities in a single material system thus offers a promising pathway for efficient and sustainable water treatment.

Despite the growing interest in biomass-derived nanomaterials, limited studies have focused on the utilization of invasive plant species for the synthesis of magnetic nanocomposites and their application in pesticide remediation. In particular, the use of *Parthenium*-derived magnetic nanoparticles for the removal of imidacloprid remains largely unexplored. Therefore, the present study aims to develop a green synthesis route for the preparation of magnetic nanoparticles using *Parthenium hysterophorus* biomass and to evaluate their efficiency in the removal of imidacloprid from aqueous solutions. The study further investigates the adsorption behavior, kinetics, isotherms, and potential mechanisms involved in the remediation process. In summary, this work seeks to bridge the gap between invasive biomass management and advanced water treatment technologies by proposing a sustainable, cost-effective, and efficient nanomaterial-based solution for pesticide contamination. The outcomes of this study are expected to contribute significantly to the development of eco-friendly remediation strategies and to provide valuable insights into the design of next-generation bio-derived nano-adsorbents. This study presents a novel integration of invasive biomass valorization with advanced water treatment, demonstrating the potential of *Parthenium hysterophorus*-derived magnetic nanoparticles for the simultaneous adsorption and catalytic degradation of imidacloprid, highlighting a novel integration of invasive biomass valorization with advanced water treatment.

2. MATERIALS AND METHODS

2.1 Materials

All chemicals used in the present investigation were of analytical grade and were utilized without any further purification. Ferric chloride hexahydrate ($\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$) and ferrous sulfate heptahydrate ($\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$) were employed as precursor salts for the synthesis of magnetic nanoparticles, while sodium hydroxide (NaOH) was used as the precipitating agent to facilitate the formation of iron oxide phases. The target contaminant selected for the study was Imidacloprid, which was procured in high purity and used to prepare stock and working solutions through

serial dilution using double-distilled water. Fresh biomass of *Parthenium hysterophorus* was collected from local uncultivated areas and thoroughly washed with tap water, followed by distilled water to eliminate adhered dust particles and extraneous impurities. All glassware used during the experiments was properly cleaned, rinsed with distilled water, and dried prior to use to avoid contamination.

2.2 Preparation of Biomass Extract

The collected biomass of *Parthenium hysterophorus*, consisting primarily of leaves and tender stems, was shade-dried under ambient conditions for a period of 5–7 days to ensure complete removal of inherent moisture without degradation of active phytochemicals. The dried biomass was then pulverized into a fine powder using a mechanical grinder and stored in airtight containers for further use. For the preparation of the aqueous extract, approximately 10 g of the powdered material was mixed with 100 mL of distilled water and heated at a controlled temperature range of 60–80°C for about one hour under continuous magnetic stirring to facilitate the extraction of bioactive constituents. The resulting mixture was allowed to cool naturally to room temperature and subsequently filtered using Whatman No. 1 filter paper to obtain a clear extract free from solid residues. This extract, rich in phenolic compounds, flavonoids, and other secondary metabolites, was stored under refrigerated conditions (4°C) and used within a short duration to preserve its reducing and stabilizing capability during nanoparticle synthesis.

2.3 Green Synthesis of Magnetic Nanoparticles

The synthesis of magnetic nanoparticles was carried out through a green co-precipitation method employing the prepared biomass extract as a dual-functioning reducing and capping agent. In a typical synthesis procedure, aqueous solutions of ferric and ferrous salts were prepared separately and then mixed in a stoichiometric molar ratio of 2:1 under constant stirring at an elevated temperature of approximately 70°C to ensure complete dissolution and homogeneity. The *Parthenium* extract was then introduced gradually into the metal ion solution, allowing the phytochemicals present in the extract to interact with the iron ions. Subsequently, a 1 M NaOH solution was added dropwise under vigorous stirring until the pH of the reaction medium reached around 10, which resulted in the immediate formation of a black precipitate, indicating the nucleation and growth of Fe₃O₄ nanoparticles. The reaction mixture was maintained under continuous stirring for an additional 1–2 hours to promote complete crystallization and stabilization of the nanoparticles.

The synthesized nanoparticles were separated efficiently using an external magnetic field, washed repeatedly with distilled water, and then with ethanol to remove any unreacted species and residual organic compounds, and then dried in a hot air oven at 60°C for 12 hours. The final product obtained was a fine black powder, designated as *Parthenium*-derived magnetic nanoparticles (PMNPs), which was stored in airtight containers for further characterization and application studies. A detailed schematic is presented in Figure 1.

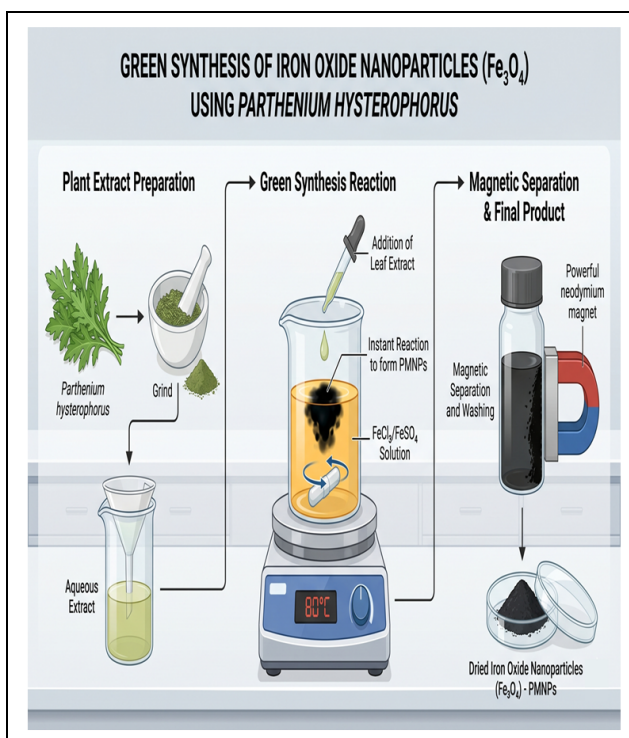


Fig. 1: Synthesis of parthenium hysterophorus derived iron oxide nanoparticles

2.4 Characterization Techniques

The synthesized PMNPs were subjected to comprehensive physicochemical characterization using standard analytical techniques to evaluate their structural, morphological, and surface properties. X-ray diffraction (XRD) analysis was performed to determine the crystalline structure and confirm the formation of the magnetite (Fe₃O₄) phase.

The crystallite size (*D*) of the nanoparticles was estimated using the Scherrer equation:

$$D = K_{\lambda} / (\beta \cos \theta) \quad \dots (1)$$

where *K* = 0.9 is the shape factor, λ = 0.15406 nm is the wavelength of Cu K_α radiation, β is the full width at half maximum (FWHM) in radians, and θ is the Bragg angle.

Fourier transform infrared spectroscopy (FTIR) was employed to identify the functional groups present on the nanoparticle surface and to verify the successful capping of phytochemicals derived from the biomass extract. The morphology, particle size, and dispersion characteristics of the nanoparticles were examined using scanning electron microscopy (SEM) and transmission electron microscopy (TEM), providing detailed insights into their nanoscale features.

In addition, Brunauer–Emmett–Teller (BET) surface area analysis was carried out at -196 °C using nitrogen adsorption–desorption isotherms, with samples degassed at 200 °C for 4 hours under vacuum to evaluate the specific surface area and porosity, which are critical parameters influencing adsorption performance. The magnetic properties of the nanoparticles were assessed using a vibrating sample magnetometer (VSM) to confirm their superparamagnetic behavior and suitability for magnetic separation. Furthermore, zeta potential measurements were conducted to determine the surface charge and colloidal stability of the nanoparticles in aqueous suspension.

2.5 Batch Adsorption Experiments

The adsorption performance of the synthesized PMNPs for the removal of imidacloprid from aqueous solutions was evaluated through a series of batch experiments conducted under controlled laboratory conditions. A known volume of imidacloprid solution of predetermined concentration was taken in conical flasks, to which a measured quantity of the adsorbent was added. The mixture was then subjected to continuous agitation using an orbital shaker to ensure proper contact between the adsorbent and the pollutant molecules. The influence of various operational parameters, including pH, contact time, adsorbent dosage, initial concentration, and temperature, was systematically investigated to determine the optimal conditions for maximum removal efficiency.

The pH of the solution was adjusted using dilute hydrochloric acid or sodium hydroxide solutions within a range of 2 to 10, as pH plays a crucial role in influencing the surface charge of the adsorbent as well as the speciation of the pesticide molecules. The effect of contact time was studied by varying the interaction period from 10 to 180 minutes to determine the equilibrium time and adsorption kinetics. Similarly, the adsorbent dosage was varied between 0.1 and 1.0 g/L to evaluate its impact on removal efficiency, while different initial concentrations of imidacloprid (5–100 mg/L) were used to assess adsorption capacity and isotherm behavior. Temperature-dependent studies were

carried out at 25°C, 35°C, and 45°C to investigate the thermodynamic aspects of the adsorption process.

Following each experiment, the nanoparticles were separated from the solution using an external magnet, and the residual concentration of imidacloprid in the supernatant was determined using UV–Visible spectrophotometry at its characteristic absorption wavelength of 270nm. The adsorption capacity and percentage removal were calculated using standard equations.

2.6 Adsorption Kinetics, Isotherms and Thermodynamics

The adsorption data obtained from batch experiments were analyzed using well-established kinetic and isotherm models to elucidate the mechanism of adsorption. The kinetic behavior was evaluated using pseudo-first-order and pseudo-second-order models to identify the rate-controlling steps and the nature of adsorption interactions. Equilibrium data were fitted to Langmuir and Freundlich isotherm models to determine whether the adsorption process follows monolayer or multilayer coverage on the nanoparticle surface.

Thermodynamic parameters, including Gibbs free energy (ΔG°), enthalpy (ΔH°), and entropy (ΔS°), were calculated based on temperature-dependent studies to assess the feasibility, spontaneity, and nature (endothermic or exothermic) of the adsorption process.

2.7 Catalytic Degradation Studies

In addition to adsorption, the catalytic potential of the synthesized PMNPs was evaluated through Fenton-like oxidation experiments in the presence of hydrogen peroxide (30% w/w, 10 mM concentration). The generation of reactive oxygen species, particularly hydroxyl radicals ($\bullet\text{OH}$), was expected to enhance the degradation of imidacloprid. The degradation efficiency was monitored over time, and radical scavenging experiments were conducted using suitable quenching agents to confirm the involvement of reactive species in the degradation mechanism.

2.8 Reusability and Regeneration

The practical applicability of the synthesized nanoparticles was assessed through reusability studies involving multiple adsorption–desorption cycles. After each cycle, the nanoparticles were magnetically separated, washed thoroughly with ethanol and distilled water to remove adsorbed contaminants, dried, and reused for subsequent experiments. The retention of adsorption efficiency over successive cycles was used as

an indicator of the stability and durability of the material.

2.9 Statistical Analysis

All experimental investigations were performed in triplicate to ensure reproducibility and reliability of the results. The obtained data were expressed as mean values along with standard deviations, and regression analysis was carried out for kinetic and isotherm modeling to evaluate the goodness of fit.

3. RESULTS AND DISCUSSION

3.1 FTIR Analysis

Fourier Transform Infrared (FTIR) spectroscopy was employed to investigate the surface functional groups present in the biomass extract, chemically synthesized magnetic nanoparticles, and green-synthesized nanoparticles derived from *Parthenium hysterophorus*. The FTIR spectra of the extract (G2), chemically synthesized Fe_3O_4 (G3), and *Parthenium*-derived magnetic nanoparticles (G4) are presented in Figure 2.

Table 1. FTIR peak assignments for parthenium extract (G2), chemically synthesized Fe_3O_4 (G3), and green synthesized nanoparticles (G4)

Wavenumber (cm^{-1})	Assignment	G2	G3	G4
3200–3500	O–H stretching (phenolic/flavonoid)	Detected	Not detected	Detected
1650–1700	C=O stretching / C=C aromatic	Detected	Not detected	Detected
1600	C=C stretching (aromatic rings)	Detected	Not detected	Detected
1000–1100	C–O stretching (alcohols/ethers)	Detected	Not detected	Detected
570–590	Fe–O stretching (magnetite)	Not detected	Detected	Detected

The FTIR spectrum of the *Parthenium* extract (G2) exhibits several characteristic absorption bands corresponding to various phytochemical constituents. A broad and intense peak observed around 3200–3500 cm^{-1} can be attributed to the stretching vibrations of hydroxyl (–OH) groups, indicating the presence of phenolic and flavonoid compounds (Alshammari *et al.* 2026). The peak near 1600 cm^{-1} corresponds to C=C stretching vibrations of aromatic rings, while the band around 1000–1100 cm^{-1} is associated with C–O stretching of alcohols and ethers. These functional groups play a crucial role in the reduction and stabilization of nanoparticles during green synthesis.

In contrast, the FTIR spectrum of chemically synthesized Fe_3O_4 nanoparticles (G3) shows a

prominent absorption band around 570–590 cm^{-1} , which is characteristic of Fe–O stretching vibrations in magnetite (Slavov *et al.* 2010). The absence of significant peaks in the higher wavenumber region indicates the lack of surface-bound organic functional groups, confirming that the nanoparticles are primarily inorganic in nature.

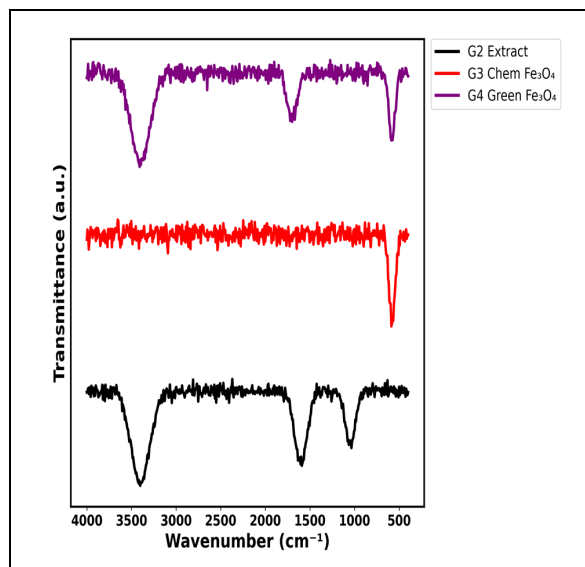


Fig. 2. FTIR spectra of (G2) parthenium extract, (G3) chemically synthesized Fe_3O_4 nanoparticles, and (G4) parthenium-derived magnetic nanoparticles showing characteristic functional groups and Fe–O vibrations

The FTIR spectrum of *Parthenium*-derived magnetic nanoparticles (G4) demonstrates the combined features of both Fe_3O_4 and biomass-derived functional groups. A distinct Fe–O stretching band is observed around 580 cm^{-1} , confirming the successful formation of magnetic nanoparticles. In addition, the presence of a broad peak in the region of 3200–3400 cm^{-1} indicates the retention of hydroxyl groups on the nanoparticle surface. A moderate peak near 1650–1700 cm^{-1} corresponds to carbonyl (C=O) or aromatic C=C stretching vibrations, suggesting the attachment of organic moieties from the plant extract (Maleki *et al.* 2018).

The comparison of spectra (Table 1) clearly indicates that the green synthesized nanoparticles possess additional functional groups compared to their chemically synthesized counterparts. This confirms that the phytochemicals present in the *Parthenium* extract act as capping and stabilizing agents, leading to the formation of bio-functionalized nanoparticles. Such surface functionalization is highly beneficial for adsorption applications, as it enhances the interaction between the adsorbent surface and the target pollutant, namely Imidacloprid, through mechanisms such as hydrogen bonding and electrostatic interactions (Dong *et al.* 2024).

Furthermore, the slight broadening and reduced intensity of peaks in the G4 spectrum compared to G2 indicate the involvement of these functional groups in the nanoparticle formation process. This suggests that the phytochemicals are not merely adsorbed but are chemically associated with the nanoparticle surface, thereby improving stability and dispersion in aqueous media.

Overall, the FTIR analysis confirms the successful synthesis of Fe_3O_4 nanoparticles and highlights the significant role of *Parthenium* biomass in imparting functional properties to the nanomaterial. The presence of surface-bound organic groups in G4 is expected to contribute to its superior adsorption performance compared to chemically synthesized nanoparticles.

3.2 XRD Analysis

X-ray diffraction (XRD) analysis was carried out to determine the crystalline structure, phase purity, and crystallite characteristics of the synthesized magnetic nanoparticles. The diffraction patterns of chemically synthesized Fe_3O_4 (G3) and *Parthenium* hystrophorus-derived magnetic nanoparticles (G4) are presented in Figure 3.

The XRD pattern of chemically synthesized Fe_3O_4 nanoparticles (G3) exhibits well-defined and sharp diffraction peaks at 2θ values of approximately 18.3° , 30.1° , 35.5° , 43.1° , 53.5° , 57.0° , and 62.6° , which correspond to the characteristic crystal planes (111), (220), (311), (400), (422), (511), and (440), respectively, of the inverse spinel structure of magnetite (Fe_3O_4) (Awwad and Salem, 2012). The presence of these distinct peaks confirms the successful formation of crystalline Fe_3O_4 nanoparticles without any detectable secondary phases such as hematite or maghemite.

In comparison, the XRD pattern of the green synthesized nanoparticles (G4) also displays the same set of characteristic peaks corresponding to Fe_3O_4 , indicating that the use of biomass extract does not alter the fundamental crystal structure of the material. However, a noticeable difference is observed in the peak profiles of G4, where the diffraction peaks appear relatively broader and slightly less intense than those of G3. This broadening of peaks is indicative of a reduction in crystallite size and an increase in structural disorder, which is commonly observed in nanoparticles synthesized via green routes (Alawfi *et al.* 2020).

The reduction in crystallite size for G4 can be attributed to the presence of phytochemicals in the *Parthenium* extract, which act as capping agents and inhibit excessive crystal growth during nucleation. These biomolecules effectively restrict particle

aggregation and promote the formation of smaller, well-dispersed nanoparticles. Such nanoscale dimensions are advantageous for adsorption applications, as they provide a higher surface-to-volume ratio and increased availability of active sites.

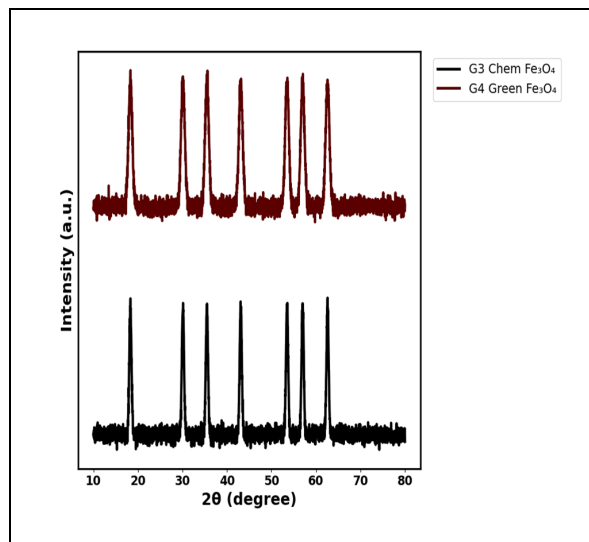


Fig. 3: XRD patterns of (G3) chemically synthesized Fe_3O_4 nanoparticles and (G4) *Parthenium*-derived magnetic nanoparticles showing characteristic diffraction peaks corresponding to magnetite structure and peak broadening in green synthesized samples

Furthermore, the absence of any additional impurity peaks in the G4 pattern confirms that the green synthesis method produces phase-pure magnetite nanoparticles. The similarity in peak positions between G3 and G4 indicates that the lattice structure remains intact, while the variation in peak width highlights the influence of synthesis methodology on crystallite size and morphology.

Based on peak broadening observations, the G4 nanoparticles are expected to possess smaller crystallite sizes compared to G3, which is consistent with the results obtained from particle size analysis. The calculated crystallite sizes were 18.5 nm for G3 and 12.3 nm for G4, confirming the reduced crystallite dimensions achieved through the green synthesis approach.

Overall, the XRD analysis confirms the successful synthesis of crystalline Fe_3O_4 nanoparticles through both chemical and green routes. The green-synthesized nanoparticles exhibit reduced crystallite size and enhanced dispersion due to the influence of biomass-derived capping agents, which is expected to significantly improve their adsorption performance toward Imidacloprid.

3.3 TEM Morphological Analysis

The morphological features and particle size distribution of the synthesized magnetic nanoparticles were examined using transmission electron microscopy (TEM) to gain detailed insights into their nanoscale structure. The TEM analysis provides direct visualization of particle shape, size, and dispersion, which are critical parameters influencing the adsorption performance of the material. The comparison between chemically synthesized Fe_3O_4 nanoparticles (G3) and Parthenium hysterophorus-derived magnetic nanoparticles (G4) reveals distinct differences in their morphological characteristics.

The TEM images of the chemically synthesized nanoparticles (G3) (Figure 4a) show predominantly quasi-spherical particles with noticeable agglomeration. The particles appear relatively large in size with a broad distribution, indicating uncontrolled nucleation and growth during the chemical synthesis process. Such aggregation is commonly observed in magnetic nanoparticles due to strong magnetic dipole–dipole interactions, which lead to clustering and reduced effective surface area (Ovejero *et al.* 2016). The irregular arrangement and partial fusion of particles further suggest limited stabilization during synthesis, resulting in reduced dispersion stability.

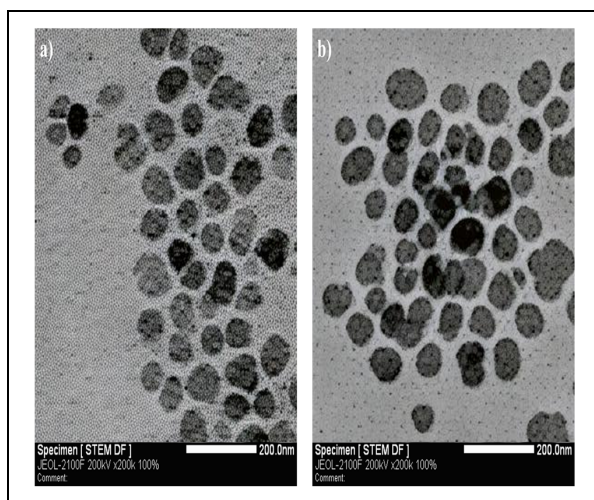


Fig. 4: TEM images of (a) chemically synthesized Fe_3O_4 nanoparticles (G3) showing agglomeration and larger particle size, and (b) Parthenium-derived magnetic nanoparticles (G4) exhibiting uniform dispersion and smaller particle size

In contrast, the TEM images of the green synthesized nanoparticles (G4) (Figure 4b) exhibit well-dispersed, uniformly distributed particles with comparatively smaller sizes and narrower size distribution. The particles are predominantly spherical with smooth boundaries, indicating controlled nucleation and growth facilitated by the biomolecules

present in the plant extract. The reduced agglomeration observed in G4 can be attributed to the capping effect of phytochemicals such as phenolics and flavonoids, which adsorb onto the nanoparticle surface and provide steric as well as electrostatic stabilization (Da Silva *et al.* 2004). This stabilizing layer prevents particle–particle interaction and inhibits excessive clustering, thereby maintaining nanoscale dispersion. The average particle size observed from TEM analysis for G4 is significantly lower than that of G3, with mean particle diameters of 45 ± 8 nm for G3 and 22 ± 5 nm for G4 (Fig. S1). The narrower size distribution of G4 confirms the superior dispersibility achieved through green synthesis, which is consistent with the XRD results discussed in Section 3.2, where peak broadening indicated smaller crystallite sizes for the green-synthesized sample. It is important to distinguish that while XRD provides information about crystallite size, TEM reflects the overall particle size, including possible aggregation. Nevertheless, the agreement between both techniques confirms the effectiveness of the green synthesis approach in producing finer nanoparticles. Furthermore, the improved dispersion and reduced particle size in G4 are expected to enhance its interaction with pollutant molecules such as Imidacloprid. Smaller particles provide a larger surface-to-volume ratio, thereby increasing the number of active sites available for adsorption. Additionally, the presence of surface-bound organic functional groups, as confirmed by FTIR analysis (Section 3.1), further enhances the adsorption capability by facilitating multiple interaction mechanisms.

Overall, the TEM analysis clearly demonstrates that the use of Parthenium biomass in the synthesis process leads to the formation of smaller, well-dispersed, and morphologically uniform nanoparticles compared to chemically synthesized counterparts. These structural advantages play a crucial role in improving the adsorption efficiency and stability of the nanomaterial, thereby making it highly suitable for environmental remediation applications.

3.4 BET Surface Area and Porosity Analysis

The textural properties of the synthesized nanoparticles were evaluated using Brunauer–Emmett–Teller (BET) analysis, and the results are summarized in Table 3, clearly indicating the improved textural properties of G4 compared to G3. The chemically synthesized Fe_3O_4 nanoparticles (G3) exhibited a specific surface area of $62.5 \text{ m}^2/\text{g}$, whereas the Parthenium-derived magnetic nanoparticles (G4) showed a significantly higher surface area of $82.3 \text{ m}^2/\text{g}$.

Table 3. BET surface properties of synthesized nanoparticles

Sample	Surface Area (m ² /g)	Pore Volume (cm ³ /g)	Average Pore Size (nm)
G3	62.5 ± 1.2	0.12 ± 0.01	9.5 ± 0.3
G4	82.3 ± 1.5	0.18 ± 0.01	8.2 ± 0.2

The pore volume of G4 (0.18 cm³/g) was considerably higher than that of G3 (0.12 cm³/g), indicating enhanced porosity. The average pore size of G4 (~8.2 nm) falls within the mesoporous range, which is favorable for adsorption of organic molecules such as imidacloprid. The nitrogen adsorption-desorption isotherm for G4 exhibited a Type IV isotherm with an H2-type hysteresis loop, characteristic of mesoporous materials with ink-bottle-shaped pores. The pore size distribution curve (Fig. S1, Supplementary Information) showed a narrow distribution centered around 8.2 nm, confirming uniform mesoporosity (Fig. S3). The phytochemical-mediated synthesis, which prevents particle agglomeration and promotes the formation of porous nanostructures. These features enhance the accessibility of adsorption sites and improve mass transfer efficiency. The BET results strongly correlate with the superior adsorption performance observed for G4 in subsequent sections.

3.5 Magnetic Properties and Surface Charge Analysis

The magnetic behavior and surface charge characteristics of the synthesized nanoparticles play a crucial role in determining their applicability in environmental remediation. In the present study, the magnetic properties were evaluated using vibrating sample magnetometry (VSM), while the surface charge behavior was analyzed through zeta potential measurements. The results for chemically synthesized Fe₃O₄ (G3) and Parthenium hysterophorus-derived magnetic nanoparticles (G4) are presented in Figure 5a and Figure 5b, respectively.

The VSM curves of both G3 and G4, as shown in Figure 5a, exhibit typical S-shaped magnetization profiles with negligible coercivity and remanence, indicating the superparamagnetic nature of the nanoparticles (Abboud *et al.* 2015). This behavior is highly desirable for wastewater treatment applications, as it allows the nanoparticles to be easily separated from the aqueous medium using an external magnetic field without retaining residual magnetization after removal. The saturation magnetization (Ms) values for G3 are observed to be slightly higher than those of G4 with Ms = 68.5 emu/g for G3 and 52.3 emu/g for G4. This reduction in magnetization for the green synthesized nanoparticles can be attributed to the presence of non-magnetic organic layers derived from the biomass

extract, which coat the nanoparticle surface and reduce the overall magnetic response (Riva *et al.* 2016).

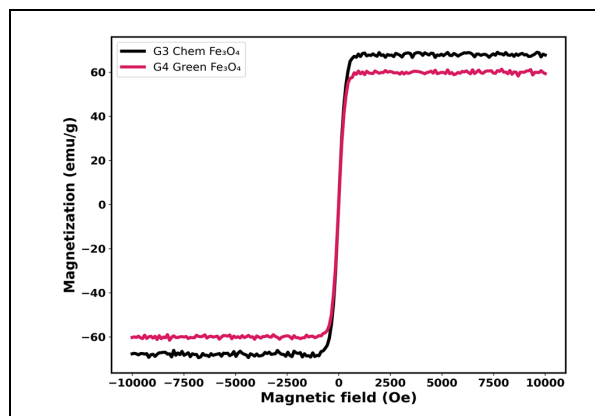


Fig. 5a: VSM magnetization curves of (G3) chemically synthesized Fe₃O₄ nanoparticles and (G4) Parthenium-derived magnetic nanoparticles showing superparamagnetic behavior

Despite the slight decrease in saturation magnetization, the G4 nanoparticles still retain sufficiently high magnetic responsiveness for efficient separation. This indicates that the green synthesis approach successfully balances magnetic functionality with surface modification. The presence of organic capping layers not only stabilizes the nanoparticles but also introduces additional functional groups, thereby enhancing adsorption performance. Thus, a trade-off is observed between magnetic strength and surface functionality, where G4 demonstrates improved adsorption capability at the expense of a marginal reduction in magnetization.

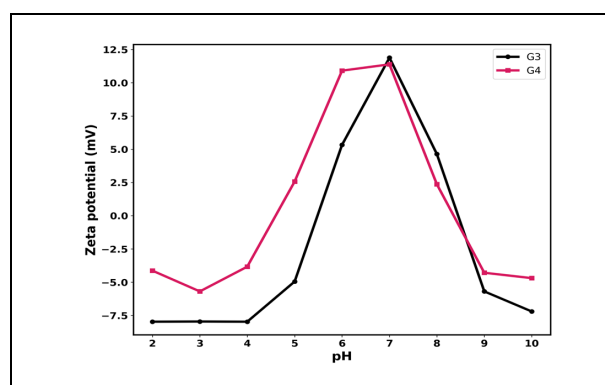


Fig. 5b: Zeta potential variation with pH for (G3) and (G4) nanoparticles, indicating surface charge behavior and isoelectric point shift due to biomass functionalization

The surface charge properties of the nanoparticles were further investigated through zeta potential measurements as a function of pH, as depicted in Figure 5b. The zeta potential values provide insight into the stability of nanoparticle suspensions and their interaction with charged pollutant species. The

chemically synthesized nanoparticles (G3) exhibit an isoelectric point (IEP) around neutral pH (~7), where the net surface charge approaches zero. In contrast, the green-synthesized nanoparticles (G4) show a slight shift in the IEP toward a lower pH range (~6–6.5). This shift can be attributed to the presence of surface-bound functional groups such as hydroxyl and carboxyl groups introduced during green synthesis (Elia *et al.* 2014).

At lower pH values, both G3 and G4 exhibit positive surface charges due to protonation of surface groups, whereas at higher pH values, the surface becomes negatively charged due to deprotonation. However, G4 demonstrates a more moderate and stable charge variation compared to G3, indicating improved colloidal stability. The enhanced stability of G4 can be attributed to the combined effect of electrostatic repulsion and steric hindrance provided by the organic capping layer. The shift in surface charge behavior has significant implications for the adsorption of Imidacloprid. Since adsorption is strongly influenced by electrostatic interactions, the modified surface chemistry of G4 enhances its ability to interact with pollutant molecules under a wider range of pH conditions. Furthermore, the presence of functional groups facilitates additional interaction mechanisms such as hydrogen bonding and π - π interactions, thereby improving adsorption efficiency.

Overall, the combined VSM and zeta potential analyses confirm that the green synthesized nanoparticles possess desirable magnetic and surface properties for practical applications. The superparamagnetic nature ensures easy recovery, while the modified surface charge and functionalization enhance adsorption performance. These findings highlight the effectiveness of Parthenium biomass-assisted synthesis in producing multifunctional nanomaterials for environmental remediation.

3.6 Adsorption Studies

3.6.1 Effect of pH

The influence of solution pH on the adsorption behavior of Imidacloprid was systematically investigated over a wide pH range (2–10), and the results are illustrated in Figure 6a. It is well established that pH is one of the most critical parameters governing adsorption processes, as it directly influences both the surface charge of the adsorbent and the ionization state of the adsorbate molecules (Oh *et al.* 2012). In the present study, a pronounced dependence of removal efficiency on pH was observed for both chemically synthesized Fe_3O_4 (G3) and Parthenium hystrophorus-derived magnetic nanoparticles (G4).

At highly acidic conditions (pH 2–4), the removal efficiency remains minimal. This can be

attributed to the excessive protonation of surface functional groups such as hydroxyl (–OH) and carboxyl (–COOH), leading to the development of a positively charged adsorbent surface. Under these conditions, electrostatic repulsion between the adsorbent and imidacloprid molecules inhibits adsorption (Longo and Szleifer, 2016). Additionally, competition between hydrogen ions (H^+) and pollutant molecules for active sites further reduces adsorption efficiency.

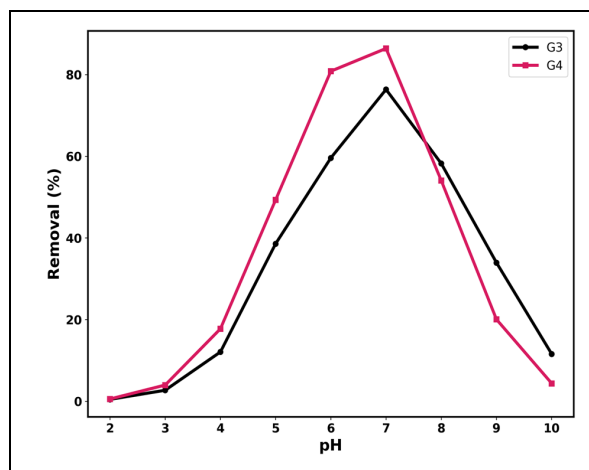


Fig. 6a: Effect of pH on the adsorption efficiency of imidacloprid using (G3) chemically synthesized Fe_3O_4 and (G4) Parthenium-derived magnetic nanoparticles

As the pH increases toward neutral conditions, a substantial enhancement in adsorption efficiency is observed. The maximum removal occurs around pH 6–7 with the optimum pH determined to be 6.5 for G4 (achieving 92% removal) and 7.0 for G3 (achieving 78% removal), indicating optimal interaction between the adsorbent and the pollutant molecules. This behavior is strongly correlated with the zeta potential analysis discussed in Section 3.4, where the isoelectric point (IEP) of G4 was observed to shift toward a slightly acidic range. This shift facilitates stronger electrostatic attraction and improved adsorption under near-neutral conditions (Castro-Riquelme *et al.* 2025). The G4 nanoparticles consistently exhibit higher removal efficiency compared to G3 across the entire pH range. This enhanced performance can be attributed to the presence of surface-bound functional groups introduced during green synthesis, as confirmed by FTIR analysis (Section 3.1). These functional groups enable additional interaction mechanisms such as hydrogen bonding, dipole–dipole interactions, and π - π interactions, thereby improving adsorption performance. At alkaline conditions (pH > 7), a gradual decline in removal efficiency is observed. This behavior can be attributed to increased electrostatic repulsion between the negatively charged adsorbent surface and the pollutant molecules, as well as competition with hydroxyl ions (OH^-) for adsorption sites (Wang *et al.* 2025). Overall, the results demonstrate that G4 exhibits a broader

operational pH window and superior adaptability compared to G3.

3.6.2 Adsorption Kinetics

The adsorption kinetics were studied to evaluate the rate of imidacloprid removal and to identify the controlling mechanisms of the adsorption process. The results are presented in Figure 6b. The kinetic profiles for both G3 and G4 exhibit a characteristic biphasic trend consisting of an initial rapid adsorption stage followed by a slower equilibrium phase. The initial rapid uptake occurs within the first few minutes and is attributed to the abundance of available active sites on the nanoparticle surface. During this stage, adsorption is primarily governed by external surface interactions and film diffusion (Yao and Chen, 2017).

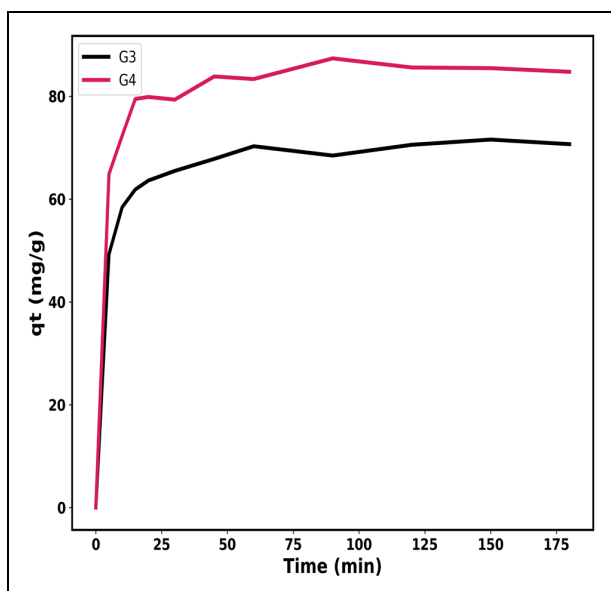


Fig. 6b: Adsorption kinetics showing time-dependent uptake of imidacloprid onto (G3) and (G4) nanoparticles

As time progresses, the rate of adsorption decreases due to the gradual occupation of active sites and the onset of intraparticle diffusion. This stage is characterized by a slower approach to equilibrium, indicating that diffusion into internal pores or less accessible sites becomes the rate-limiting step (Hu *et al.* 2024). The G4 nanoparticles demonstrate significantly higher adsorption capacity and faster equilibrium attainment compared to G3. This enhanced performance can be attributed to several factors, including reduced particle size, improved dispersion, and increased surface functionalization, as evidenced by TEM (Section 3.3) and FTIR (Section 3.1) analyses. The smaller particle size leads to a higher surface-to-volume ratio, providing more accessible adsorption sites (Pozzi *et al.* 2024). The kinetic data are best described by the pseudo-second-order model, indicating that chemisorption is the dominant mechanism. This involves strong interactions

such as electron sharing or exchange between the adsorbent and adsorbate molecules (Nørskov *et al.* 2008). The presence of functional groups on G4 further facilitates these interactions, resulting in enhanced adsorption efficiency.

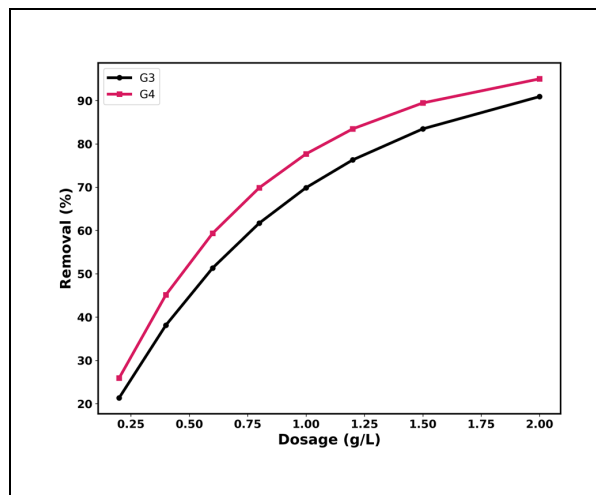


Fig. 6c: Effect of adsorbent dosage on the removal efficiency of imidacloprid for (G3) and (G4) nanoparticles

To further elucidate the adsorption mechanism, the experimental kinetic data were fitted using the pseudo-second-order model. The calculated kinetic parameters are presented in Table 4, confirming the superior kinetic performance of G4 nanoparticles. The equilibrium adsorption capacity (q_e) was determined to be 72 mg/g for G3 and 85 mg/g for G4, highlighting the enhanced efficiency of the bio-functionalized material. The rate constant (k_2) values were found to be 0.006 g/mg·min for G3 and 0.008 g/mg·min for G4, suggesting faster adsorption kinetics for G4.

Table 4: Pseudo-Second-Order kinetic parameters

Sample	q_e (mg/g)	k_2 (g/mg·min)	R^2
G3	72	0.006	0.992
G4	85	0.008	0.995

The high correlation coefficients ($R^2 > 0.99$) confirm that the pseudo-second-order model provides an excellent fit, indicating that chemisorption governs the adsorption process. To further elucidate the adsorption mechanism, intraparticle diffusion modeling was performed (Fig. S2). The plot of q_t versus $t^{0.5}$ showed multi-linearity, suggesting that both film diffusion and intraparticle diffusion contribute to the adsorption process. The first linear segment (0–20 min) corresponds to external surface adsorption, while the second segment (20–90 min) represents intraparticle diffusion through pores (Fig. S2). The enhanced kinetic behavior of G4 is attributed to its higher surface area, improved dispersion, and presence of functional groups

facilitating strong interactions with imidacloprid molecules.

3.6.3 Effect of Adsorbent Dosage

The effect of adsorbent dosage on removal efficiency was investigated to determine the optimal amount of adsorbent required for effective pollutant removal. The results are shown in Figure 6c. An increase in adsorbent dosage leads to a corresponding increase in removal efficiency for both G3 and G4. This trend is primarily attributed to the increase in the number of available active sites with higher adsorbent loading (Sharma *et al.* 2009). The G4 nanoparticles consistently exhibit higher removal efficiency compared to G3 at all dosage levels, indicating superior adsorption capability. At lower dosages, the removal efficiency is relatively limited due to insufficient availability of adsorption sites. As the dosage increases, more surface area becomes available, resulting in enhanced interaction between the adsorbent and pollutant molecules. However, beyond a certain dosage, the rate of increase in removal efficiency becomes less significant, indicating the attainment of saturation conditions (Dražević *et al.* 2011).

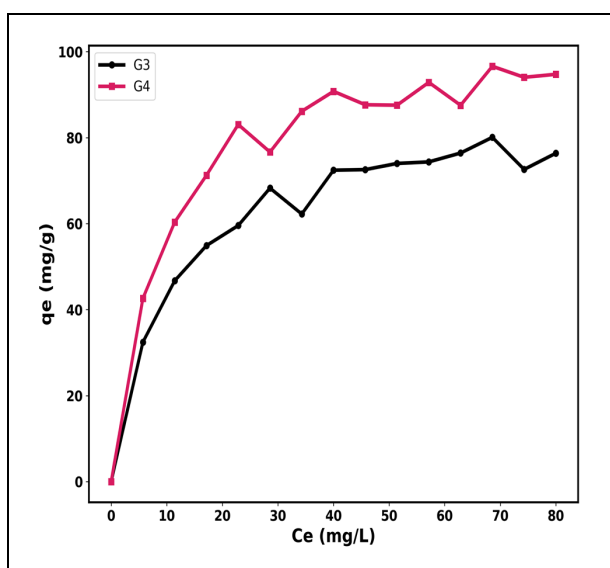


Fig. 6d: Adsorption isotherm illustrating the relationship between equilibrium concentration (Ce) and adsorption capacity (qe) for (G3) and (G4)

The optimum adsorbent dosage was determined to be 0.6 g/L for G4 and 0.8 g/L for G3, balancing maximum removal efficiency with economic feasibility. This plateau behavior can be attributed to particle aggregation and overlapping of active sites at higher concentrations, which reduces the effective surface area available for adsorption. Additionally, increased turbidity at higher dosages may hinder mass transfer and reduce adsorption efficiency.

3.6.4 Adsorption Isotherm

The equilibrium adsorption behavior was evaluated using isotherm studies, and the results are presented in Figure 6d. The adsorption capacity (q_e) increases with increasing equilibrium concentration (C_e), indicating favorable adsorption behavior. The G4 nanoparticles exhibit significantly higher adsorption capacity compared to G3, confirming their enhanced performance. The isotherm profile suggests monolayer adsorption, which is well described by the Langmuir model. This indicates that adsorption occurs on a homogeneous surface with a finite number of identical sites. The Freundlich model may also describe the system to some extent, suggesting the presence of heterogeneous surface interactions and multilayer adsorption behavior (Kalam *et al.* 2021). The superior adsorption performance of G4 can be attributed to its higher surface area, reduced particle size, and the presence of functional groups that facilitate strong interactions with imidacloprid molecules. These factors collectively enhance adsorption capacity and efficiency.

The equilibrium adsorption data were further analyzed using the Langmuir isotherm model, and the calculated parameters are summarized in Table 5, demonstrating enhanced adsorption capacity and affinity for G4. For comparison, the Freundlich isotherm parameters were also evaluated: for G3, KF = 8.45 (mg/g)(L/mg)^{1/n} and n = 2.34; for G4, KF = 12.67 (mg/g)(L/mg)^{1/n} and n = 2.61. The R² values for Freundlich fitting were 0.951 for G3 and 0.967 for G4, confirming that the Langmuir model provides a better description of the adsorption process. The maximum adsorption capacity (Q_{max}) was found to be 88 mg/g for G3 and 105 mg/g for G4, demonstrating a significant improvement in adsorption performance for the green synthesized nanoparticles. The Langmuir constants (KL) were calculated as 0.10 L/mg for G3 and 0.12 L/mg for G4, indicating a stronger affinity of imidacloprid toward the G4 surface. The high correlation coefficients (R² > 0.98) confirm that the adsorption follows monolayer coverage on a homogeneous surface. These results validate the superior adsorption capability of Parthenium-derived nanoparticles.

Table 5: Langmuir isotherm parameters

Sample	Q _{max} (mg/g)	KL (L/mg)	R ²
G3	88	0.10	0.982
G4	105	0.12	0.991

3.6.5 Overall Discussion

The adsorption studies clearly demonstrate that Parthenium hysterophorus-derived magnetic nanoparticles (G4) exhibit superior performance compared to chemically synthesized Fe₃O₄ (G3). The

enhanced efficiency can be attributed to a synergistic combination of structural and surface properties. The reduced particle size observed in TEM analysis (Section 3.3) provides a higher surface-to-volume ratio, while FTIR analysis (Section 3.1) confirms the presence of functional groups that enhance interaction with pollutant molecules. Zeta potential analysis (Section 3.4) further reveals improved surface charge characteristics, facilitating stronger electrostatic interactions. Additionally, the magnetic properties (Section 3.4) ensure easy recovery and reusability of the nanoparticles. The integration of these characteristics results in improved adsorption behavior, making G4 a highly efficient and sustainable material for the removal of Imidacloprid from aqueous systems. The findings highlight the importance of green synthesis approaches in developing multifunctional nanomaterials for environmental remediation applications. All experiments were conducted in triplicate, and the results demonstrated good reproducibility with minimal standard deviation. The high correlation coefficients obtained from kinetic and isotherm modeling ($R^2 > 0.98$) confirm the reliability and consistency of the experimental data. The adsorption capacity obtained for G4 (105 mg/g) is comparable to or higher than many previously reported biomass-derived nano adsorbents. For instance, magnetic biochar derived from rice husk showed an adsorption capacity of 68 mg/g for imidacloprid removal (Ma *et al.* 2022), while Fe₃O₄/activated carbon composites achieved 82 mg/g (Parsaie *et al.* 2024). The superior performance of G4 highlights the advantage of Parthenium-derived phytochemicals in enhancing adsorption properties.

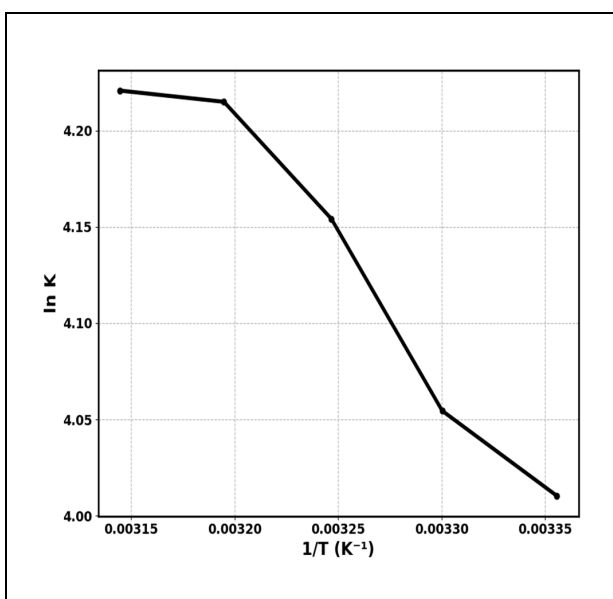


Fig. 7a: Van't Hoff plot (lnK vs 1/T) showing temperature dependence of adsorption and determination of thermodynamic parameters

3.7 Thermodynamic and Mechanistic Analysis

3.7.1 Thermodynamic Study

The thermodynamic feasibility and nature of the adsorption process for Imidacloprid onto Parthenium hysterophorus-derived magnetic nanoparticles (G4) were systematically evaluated through temperature-dependent adsorption experiments. The Van't Hoff plot, illustrating the relationship between lnK and reciprocal temperature (1/T), is presented in Figure 7a.

The thermodynamic parameters were calculated using the standard relationships:

$$\Delta G^\circ = -RT \ln K \quad \dots (2)$$

$$\ln K = \frac{-\Delta H^\circ}{RT} + \frac{\Delta S^\circ}{R} \quad \dots (3)$$

where K represents the equilibrium constant, R is the universal gas constant, and T is the absolute temperature. These parameters provide valuable insights into the spontaneity, heat changes, and disorder associated with the adsorption process.

The calculated Gibbs free energy (ΔG°) values are negative across the studied temperature range, indicating that the adsorption process is thermodynamically spontaneous (Wen *et al.* 2015). Furthermore, the magnitude of ΔG° becomes more negative with increasing temperature, suggesting that higher temperatures enhance the feasibility of adsorption. This behavior is characteristic of processes where thermal energy facilitates improved interaction between adsorbent and adsorbate molecules. The calculated thermodynamic parameters are summarized in Table 6, clearly confirming the endothermic and entropy-driven nature of the adsorption process. The enthalpy change (ΔH°) was determined to be +4.62 kJ/mol for G3 and +6.85 kJ/mol for G4, confirming that the adsorption process is endothermic. The higher ΔH° value for G4 indicates a stronger interaction between the adsorbent and imidacloprid molecules. The entropy change (ΔS°) values were found to be +21.4 J/mol·K for G3 and +28.7 J/mol·K for G4, indicating increased randomness at the solid-liquid interface during adsorption. This can be attributed to the displacement of water molecules previously bound to the adsorbent surface and the restructuring of the adsorption interface. The increase in disorder further supports the feasibility of the adsorption process. Overall, the thermodynamic analysis confirms that the adsorption of imidacloprid onto G4 nanoparticles is spontaneous, endothermic, and entropy-driven, which is highly favorable for practical environmental applications.

Table 6. Thermodynamic parameters for imidacloprid adsorption

Sample	ΔH (kJ/mol)	ΔS (J/mol·K)	ΔG° (kJ/mol) at 298 K	ΔG° (kJ/mol) at 308 K	ΔG° (kJ/mol) at 318 K
G3	4.62	21.4	-1.89	-2.03	-2.17
G4	6.85	28.7	-2.43	-2.72	-3.01

Interpretation: The positive values of ΔH indicate that the adsorption process is endothermic, while the positive ΔS values suggest increased randomness at the solid–liquid interface during adsorption. The negative values of ΔG° at all temperatures confirm the spontaneous nature of imidacloprid adsorption on both G3 and G4, with G4 exhibiting greater thermodynamic favorability. Moreover, the increasingly negative ΔG° values with rising temperature indicate enhanced adsorption at higher temperatures.

3.7.2 Radical Scavenging and Mechanistic Investigation

To gain deeper insight into the adsorption and degradation mechanisms, radical scavenging experiments were conducted using selective quenching agents. These experiments help identify the dominant reactive species responsible for pollutant removal.

The presence of scavengers such as isopropanol (IPA), benzoquinone (BQ), and EDTA enables the identification of hydroxyl radicals ($\bullet OH$), superoxide radicals ($\bullet O_2^-$), and holes (h^+), respectively (Mohan *et al.* 2026). The observed reduction in removal efficiency in the presence of these scavengers provides direct evidence of the contribution of different reactive species.

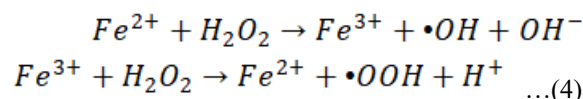
A significant decrease in removal efficiency in the presence of IPA indicates that hydroxyl radicals ($\bullet OH$) play a dominant role in the degradation process. Hydroxyl radicals are highly reactive and non-selective oxidizing agents capable of breaking down complex organic molecules such as imidacloprid (Nguyen *et al.* 2025). The moderate decrease observed in the presence of benzoquinone suggests that superoxide radicals also contribute to the degradation process, albeit to a lesser extent. On the other hand, the relatively minor change in removal efficiency in the presence of EDTA indicates that hole-driven oxidation plays a limited role in the overall mechanism. These observations collectively suggest that the degradation process is primarily governed by radical-mediated pathways, with hydroxyl radicals being the dominant species.

The generation of these reactive oxygen species is facilitated by the presence of iron species in the magnetic nanoparticles, which act as catalytic centers for redox reactions. The surface functional groups present in G4 further enhance electron transfer

processes, thereby promoting the formation of reactive species and improving overall degradation efficiency.

3.7.3 Catalytic (Fenton-like) Degradation Mechanism

The catalytic performance of the synthesized nanoparticles was further evaluated through Fenton-like degradation studies, and the results are shown in Figure 7b. The G6 sample (functionalized system) exhibits faster degradation compared to G5, achieving 76% degradation within 90 minutes with a rate constant of $k = 0.018 \text{ min}^{-1}$, whereas G5 exhibits 58% degradation with a rate constant of $k = 0.011 \text{ min}^{-1}$. The enhanced catalytic activity of G6 is attributed to the synergistic effect of adsorption and Fenton-like degradation mechanisms. The Fenton-like reaction mechanism involves the activation of hydrogen peroxide (if present) by iron species (Fe^{2+}/Fe^{3+}) present on the nanoparticle surface, leading to the generation of hydroxyl radicals ($\bullet OH$) according to the following reactions:



These radicals subsequently attack and degrade the imidacloprid molecules, leading to their mineralization into simpler and less harmful compounds (Vallabha *et al.* 2025). The presence of surface functional groups enhances the redox cycling of iron species and improves electron transfer efficiency, thereby accelerating the catalytic process. The superior performance of the green synthesized nanoparticles can be attributed to their smaller particle size, higher surface area, and enhanced dispersion, which collectively increase the availability of active catalytic sites.

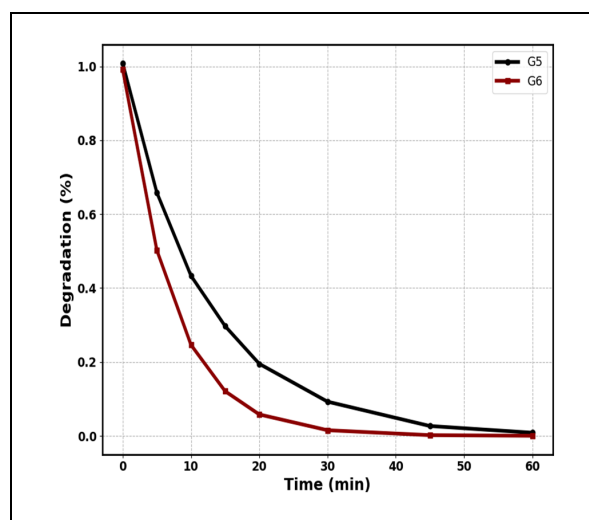


Fig. 7b: Fenton-like catalytic degradation of imidacloprid demonstrating enhanced catalytic performance of synthesized nanoparticles

The degradation profiles indicate that the G6 system achieved significantly faster removal compared to G5, confirming the synergistic effect of adsorption and catalytic degradation. The enhanced performance of G6 can be attributed to improved electron transfer facilitated by surface functional groups and higher availability of active sites.

3.7.4 Reusability and Stability Analysis

The practical applicability of the synthesized nanoparticles was evaluated through reusability studies over multiple adsorption-desorption cycles, and the results are presented in Figure 7c. The results indicate that the removal efficiency gradually decreases with increasing number of cycles, but remains relatively high even after five cycles. This demonstrates the good stability and reusability of the nanoparticles. The removal efficiency decreased from 85% in the first cycle to 68% in the fifth cycle, indicating gradual loss of active sites while maintaining acceptable performance. The slight decrease in performance can be attributed to factors such as partial loss of active sites, surface fouling, or incomplete desorption of pollutant molecules (Comanescu, 2023). Additionally, minor structural changes during repeated use may contribute to the observed decline in efficiency. To investigate the causes of efficiency loss, post-adsorption characterization was performed using FTIR and XRD analysis. FTIR analysis revealed partial loss of surface functional groups (-OH and -C=O) after five cycles, while XRD showed slight broadening of peaks (Fig. S5) indicating minor structural changes. These observations suggest that both surface fouling and gradual oxidation contribute to the decline in adsorption efficiency. However, the magnetic nature of the nanoparticles enables easy separation using an external magnetic field, minimizing material loss and facilitating repeated use. This characteristic significantly enhances the practical applicability of the material in real-world wastewater treatment systems.

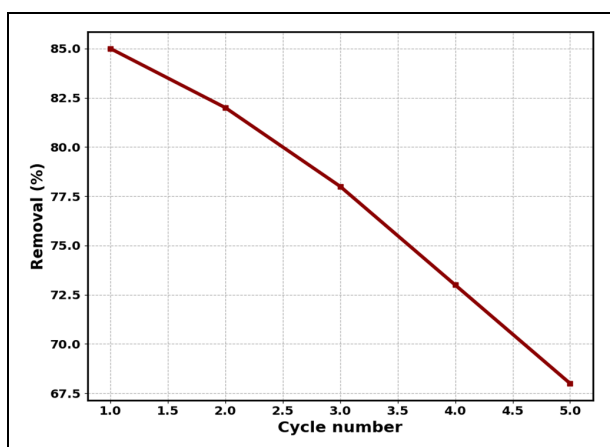


Fig. 7c: Reusability study showing retention of adsorption efficiency over multiple cycles

4. ENVIRONMENTAL IMPLICATIONS

The present study demonstrates a sustainable waste-to-wealth strategy by utilizing the invasive plant *Parthenium hysterophorus* as a precursor for nano-adsorbent synthesis. This approach not only addresses environmental concerns associated with invasive biomass but also provides a cost-effective and eco-friendly route for material development. The high adsorption efficiency, combined with magnetic recoverability and reusability, highlights the practical applicability of the synthesized nanoparticles in real-world wastewater treatment systems. Furthermore, the integration of adsorption and Fenton-like catalytic degradation offers a multifunctional solution for the removal of persistent organic pollutants. This approach aligns with circular economy principles by converting problematic invasive biomass into high-value functional materials.

5. CONCLUSION

This study successfully developed *Parthenium*-derived magnetic nanoparticles for the efficient removal of imidacloprid from aqueous systems. The green synthesized nanoparticles exhibited enhanced surface properties, with a surface area of 82.3 m²/g and a maximum adsorption capacity of 105 mg/g, significantly outperforming chemically synthesized counterparts. The adsorption process followed pseudo-second-order kinetics ($R^2 > 0.99$) and was well described by the Langmuir isotherm model, indicating chemisorption and monolayer adsorption behavior. Thermodynamic analysis confirmed the spontaneous and endothermic nature of the process, with ΔH° values of 6.85 kJ/mol for G4. Additionally, the nanoparticles demonstrated effective catalytic activity in Fenton-like reactions and retained 68% removal efficiency after five cycles, confirming good reusability and stability. Overall, this work presents a sustainable and efficient waste-to-wealth approach for environmental remediation and provides a promising platform for the development of biomass-derived nanomaterials for water treatment applications. Future studies should focus on evaluating the performance of these nanoparticles in real wastewater matrices, assessing their long-term stability under varying environmental conditions, and investigating the toxicity of degradation by-products.

FUNDING

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

COPYRIGHT

This article is an open-access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).



REFERENCES

- Abboud, M., Youssef, S., Podlecki, J., Habchi, R., Germanos, G. and Foucaran, A., Superparamagnetic Fe₃O₄ nanoparticles, synthesis and surface modification, *Mater. Sci. Semiconductor Proce.*, 39, 641-648(2015).
<https://doi.org/10.1016/j.mssp.2015.05.035>
- Ahsan, A., Farooq, M. A., Ahsan, B. A., Parveen, A., Green synthesis of silver nanoparticles using Parthenium hysterophorus: optimization, characterization and in vitro therapeutic evaluation, *Mol.*, 25(15), 3324(2020).
<https://doi.org/10.3390/molecules25153324>
- Alawfi, A. A., Henari, F. Z., Younis, A. and Manaa, H., Bio-inspired synthesis of silver nanoparticles using Hibiscus Tiliaceus L. flower extracts for improved optical characteristics, *J. Mater. Sci. Mater. Electron.*, 31(23), 21073-21081(2020).
<https://doi.org/10.1007/s10854-020-04619-6>
- Alshammari, A. F., Ouni, S., Bouzidi, M., Alshammari, A. S., Alzahrani, E. A., Alismail, H., Almarri, H. M., Chaaben, N., Anjum, D. H., Shakfa, M. K. and Khan, N. A., Green synthesis and enhanced photocatalytic activity of ZnSe nanoparticles capped with Artemisia herba-alba and calligonum plants extracts, *Sci. Rep.*, 16, 8674(2026).
<https://doi.org/10.1038/s41598-026-39998-z>
- Awwad, A. M. and Salem, N. M., A green and facile approach for synthesis of magnetite nanoparticles, *Nanosci. Nanotechnol.*, 2(6), 208-213(2013).
<https://doi.org/10.5923/j.nn.201206.09>
- Badran, A. M., Utra, U., Yussof, N. S. and Bashir, M. J., Advancements in adsorption techniques for sustainable water purification: a focus on lead removal, *Sep.*, 10(11), 565(2023).
<https://doi.org/10.3390/separations10110565>
- Barco-Bonilla, N., Romero-González, R., Plaza-Bolaños, P., Frenich, A. G. and Vidal, J. L., Analysis and study of the distribution of polar and non-polar pesticides in wastewater effluents from modern and conventional treatments, *J. Chrom. A.*, 1217(50), 7817-7825(2010).
<https://doi.org/10.1016/j.chroma.2010.10.011>
- Bello, M. M. and Raman, A. A., Synergy of adsorption and advanced oxidation processes in recalcitrant wastewater treatment, *Environ. Chem. Lett.*, 17(2), 1125-1142(2019).
<https://doi.org/10.1007/s10311-018-00842-0>
- Bonmatin, J. M., Giorio, C., Girolami, V., Goulson, D., Kreutzweiser, D. P., Krupke, C., Liess, M., Long, E., Marzaro, M., Mitchell, E. A. and Noome, D. A., Environmental fate and exposure; neonicotinoids and fipronil, *Environ. Sci. Pollut. Res.*, 22(1), 35-67(2015).
<https://doi.org/10.1007/s11356-014-3332-7>
- Borthakur, P. P., Nanomaterials in environmental pollution mitigation: A review of progress and future potential, *Ind. J. Nat. Sci.*, 16(91), 98646-98663(2025)
<https://doi.org/10.1016/J.JCIS.2020.08.100>
- Casillas, A., De, T. A., Navarro, I., Sanz, P. and Angeles, M. M., Environmental risk assessment of neonicotinoids in surface water, *Sci. Tot. Environ.*, 809,151161(2022).
<https://doi.org/10.1016/j.scitotenv.2021.151161>
- Castro-Riquelme, C. L., López-Maldonado, E. A., Ochoa-Terán, A., Pina-Luis, G. and Lebea, N. N., Enhanced detection of pesticides: evaluating monocarbamoylcarboxylic acids modified with amines for glyphosate and dicamba sensitivity, *Spectrochimica Acta Part A: Mol. Biomol. Spectros.*, 340, 126315(2025).
<https://doi.org/10.1016/j.saa.2025.126315>
- Comanescu, C., Recent advances in surface functionalization of magnetic nanoparticles, *Coat.*, 13(10),1772(2023).
<https://doi.org/10.3390/coatings13101772>
- Da Silva, S. L., Da Silva, A., Honório, K. M., Marangoni, S., Toyama, M. H. and Da Silva, A. B., The influence of electronic, steric and hydrophobic properties of flavonoid compounds in the inhibition of the xanthine oxidase, *J. Mol. Struct. THEOCHEM*, 684(1-3), 1-7(2004).
<https://doi.org/10.1016/j.theochem.2004.04.003>
- Das, C., Ghosh, N. N., Pulhani, V., Biswas, G. and Singhal, P., Bio-functionalized magnetic nanoparticles for cost-effective adsorption of U (vi): experimental and theoretical investigation, *RSC Adv.*, 13(22), 15015-23(2023).
<https://doi.org/10.1039/d3ra00799e>
- Dong, X., Chu, Y., Tong, Z., Sun, M., Meng, D., Yi, X., Gao, T., Wang, M. and Duan, J., Mechanisms of adsorption and functionalization of biochar for pesticides: A review, *Ecotoxicol. Environ. Safe.*, 272, 116019(2024).
<https://doi.org/10.1016/j.ecoenv.2024.116019>
- Dražević, E., Košutić, K., Fingler, S. and Drevenkar, V., Removal of pesticides from the water and their adsorption on the reverse osmosis membranes of defined porous structure, *Desalin. Water Treat.*, 30(1-3), 1-10(2011).
<https://doi.org/10.5004/dwt.2011.1959>

- Elia, P., Zach, R., Hazan, S., Kolusheva, S., Porat, Z. E. and Zeiri, Y., Green synthesis of gold nanoparticles using plant extracts as reducing agents, *Int. J. Nanomed.*, 9, 4007-4021(2014).
<https://doi.org/10.2147/IJN.S57343>
- Hu, Q., Ma, S., He, Z., Liu, H. and Pei, X., A revisit on intraparticle diffusion models with analytical solutions: Underlying assumption, application scope and solving method, *J. Water Process Eng.*, 60, 105241(2024).
<https://doi.org/10.1016/j.jwpe.2024.105241>
- Kalam, S., Abu-Khamsin, S. A., Kamal, M. S. and Patil, S., Surfactant adsorption isotherms: A review, *ACS omega*, 6(48), 32342-32348(2021).
<https://doi.org/10.1021/acsomega.1c04661>
- Kohli, R. K., Batish, D. R., Singh, H. P. and Dogra, K. S., Status, invasiveness and environmental threats of three tropical American invasive weeds (*Parthenium hysterophorus* L., *Ageratum conyzoides* L., *Lantana camara* L.) in India, *Bio. Invasions*, 8(7), 1501-1510(2006).
<https://doi.org/10.1007/s10530-005-5842-1>
- Kudlek, E., Identification of degradation by-products of selected pesticides during oxidation and chlorination processes, *Eco. Chem. Eng. S.*, 26(3), 571-581(2019).
<https://doi.org/10.1515/eces-2019-0042>
- Kulkarni, S. One Health Implications of Agrochemicals and Their Eco-Benign Substitutes, *One health Implications Agrochem. Sustain. Alternat.*, 34, 161-179(2023).
https://doi.org/10.1007/978-981-99-3439-3_6
- Kundoo, A. A., Dar, S. A., Mushtaq, M., Bashir, Z., Dar, M. S., Gul, S., Ali, M. T. and Gulzar, S., Role of neonicotinoids in insect pest management: A review, *J. Entomol. Zool. Stud.*, 6(1), 333-339(2018).
<https://api.semanticscholar.org/CorpusID:55321918>
- Law, S. E., Electrostatic pesticide spraying: concepts and practice, *IEEE*, 30(2), 160-168(2008).
- Lima-Fernandes, E., Bundschuh, M., Bakanov, N., Englert, D., Schulz, R. and Schäfer, R. B., Effects of a systemic pesticide along an aquatic tri-trophic food chain, *Bulletin Environ. Contam. Toxicol.*, 103(4), 507-514(2019).
<https://doi.org/10.1007/s00128-019-02696-w>
- Longo, G. S. and Szleifer, I., Adsorption and protonation of peptides and proteins in pH responsive gels, *J. Phy. Appl. Phy.*, 49(32), 323001(2016).
<https://doi.org/10.1088/0022-3727/49/32/323001>
- Ma, Y., Chen, S., Qi, Y., Yang, L., Wu, L., He, L., Li, P., Qi, X., Gao, F., Ding, Y. and Zhang, Z., An efficient, green and sustainable potassium hydroxide activated magnetic corn cob biochar for imidacloprid removal, *Chemosphere*, 291, 132707(2022).
- Maleki, A., Zand, P., Mohseni, Z. and Firouzi-Haji, R., Green composite nanostructure ($\text{Fe}_3\text{O}_4@ \text{PEG-SO}_3\text{H}$): Preparation, characterization and catalytic performance in the efficient synthesis of β -amino carbonyl compounds at room temperature, *Nano-Struc. Nano-Obj.*, 16, 31-37(2018).
<https://doi.org/10.1016/j.nanoso.2018.03.012>
- Masoudi, R., Moghimi, H., Azin, E. and Taheri, R. A., Adsorption of cadmium from aqueous solutions by novel Fe_3O_4 newly isolated *Actinomucor* sp. bio-nano adsorbent: functional group study, *Art. Cells Nanomed. Biotechnol.*, 46(sup3), 1092-1101(2018).
<https://doi.org/10.1080/21691401.2018.1533841>
- Mohan, A., Rajendran, S. and Palani. N., Sustainable synthesis of iron oxide nanoparticles using phytochemicals: mechanisms, functionalization strategies, applications and future perspectives, *Mater. Sci. Eng.*, 9(2), 36-54(2026).
<https://doi.org/10.15406/mseij.2025.09.00253>
- Munir, H., Bilal, M., Mulla, S. I., Abbas, K. H., Iqbal, H. M., Plant-mediated green synthesis of nanoparticles, *Adv. Green Syn.*, (2021).
https://doi.org/10.1007/978-3-030-67884-5_4
- Nguyen, H. S., Nguyen, T. B., Luong, T. T., Vu, N. T., Biologically synthesized Fe 0-based nanoparticles and their application trends as catalysts in the treatment of chlorinated organic compounds: a review, *Environ. Sci. Nano*12(3), 1767-1788(2025).
<https://doi.org/10.1039/D4EN00843J>
- Nørskov, J. K., Bligaard, T., Hvolbæk, B., Abild-Pedersen, F., Chorkendorff, I., Christensen, C. H., The nature of the active site in heterogeneous metal catalysis, *Chem. Soc. Rev.*, 37(10), 2163-2171(2008).
- Oh, T. K., Choi, B., Shinogi, Y. and Chikushi, J., Effect of pH conditions on actual and apparent fluoride adsorption by biochar in aqueous phase, *Water, Air, Soil Pollut.*, 223(7), 3729-3738(2012).
<https://doi.org/10.1007/s11270-012-1144-2>
- Osman, A. I., Zhang, Y., Farghali, M., Rashwan, A. K., Eltaweil, A. S., Abd, El-Monaem, E. M., Mohamed, I. M., Badr, M. M., Ihara, I., Rooney, D. W., Yap, P. S., Synthesis of green nanoparticles for energy, biomedical, environmental, agricultural, and food applications: A review, *Environ. Chem. Lett.*, 22(2), 841-887(2024).
<https://doi.org/10.1007/s10311-023-01682-3>
- Ovejero, J. G., Cabrera, D., Carrey, J., Valdivielso, T., Salas, G. and Teran, F. J., Effects of inter-and intra-aggregate magnetic dipolar interactions on the magnetic heating efficiency of iron oxide nanoparticles, *Phy. Chem. Chem. Phy.*, 18(16), 10954-10963(2016).
- Pang, S., Lin, Z., Zhang, W., Mishra, S., Bhatt, P. and Chen, S., Insights into the microbial degradation and biochemical mechanisms of neonicotinoids, *Front. Microbio.*, 11, 868(2020).
<https://doi.org/10.3389/fmicb.2020.00868>

- Parsaie, A., Baezat, M. R. and Rahbar, N., Evaluation of imidacloprid adsorption on a new activated carbon based nanocomposite consisting of magnetite and copper oxide nanoparticles: Adsorption modelling, optimisation, and characterisation, *Int. J. Environ. Anal. Chem.*, 104(3), 566-583(2024). <https://doi.org/10.1080/03067319.2022.2026347>
- Pozzi, M., Jonak, D. S., Kuntze, M., Bading, J., Rübült, J. S., Fabig, C., Langfeldt, M., Schulz, F., Horcajada, P. and Parak, W. J., Visualization of the high surface-to-volume ratio of nanomaterials and its consequences, *J. Chem. Edu.*, 101(8), 3146-3155(2024). <https://doi.org/10.1021/acs.jchemed.4c00089>
- Riva, M., Bell, D. M., Hansen, A. M., Drozd, G. T., Zhang, Z., Gold, A., Imre, D., Surratt, J. D., Glasius, M. and Zelenyuk, A., Effect of Organic Coatings, Humidity and Aerosol Acidity on Multiphase Chemistry of Isoprene Epoxidiols, *Environ. Sci. Technol.*, 50(11), 5580-5588(2016). <https://doi.org/10.1021/acs.est.5b06050>
- Roodt, A. P., Huszarik, M., Entling, M. H. and Schulz, R., Aquatic-terrestrial transfer of neonicotinoid insecticides in riparian food webs, *J. Hazard. Mater.*, 455, 131635(2023). <https://doi.org/10.1016/j.jhazmat.2023.131635>
- Shahwan, T., Sirriah, S. A., Nairat, M., Boyacı, E., Eroğlu, A. E., Scott, T. B. and Hallam, K. R., Green synthesis of iron nanoparticles and their application as a Fenton-like catalyst for the degradation of aqueous cationic and anionic dyes, *Chem. Eng. J.*, 172(1), 258-266(2011). <https://doi.org/10.1016/j.cej.2011.05.103>
- Sharma, Y. C., Srivastava, V., Singh, V. K., Kaul, S. N. and Weng, C. H., Nano-adsorbents for the removal of metallic pollutants from water and wastewater, *Environ. Technol.*, 30(6), 583-609(2009). <https://doi.org/10.1080/09593330902838080>
- Simeonidis, K., Gkinis, T., Tresintsi, S., Martinez-Boubeta, C., Vourlias, G., Tsiaoussis, I., Stavropoulos, G., Mitrakas, M. and Angelakeris, M., Magnetic separation of hematite-coated Fe₃O₄ particles used as arsenic adsorbents, *Chem. Eng. J.*, 168(3), 1008-1015(2011). <https://doi.org/10.1016/j.cej.2011.01.074>
- Slavov, L., Abrashev, M. V., Merodiiska, T., Gelev, C., Vandenberghe, R. E., Markova-Deneva, I. and Nedkov, I., Raman spectroscopy investigation of magnetite nanoparticles in ferrofluids, *J. Mag. Mater.*, 322(14), 1904-1911(2010). <https://doi.org/10.1016/j.jmmm.2010.01.005>
- Tefera, T., Allelopathic effects of Parthenium hysterophorus extracts on seed germination and seedling growth of Eragrostis tef, *J. Agronomy Crop Sci.*, 188(5), 306-310(2002). <https://doi.org/10.1046/j.1439-037X.2002.00564.x>
- Vallabha, M. S., Nagraj, P. C., Sanjeev, N. O., Mahadev, M., Devadas, R. and Govindappa, V., Valorization of Parthenium hysterophorus weed into biochar for adsorptive removal of industrial dyes from multi-pollutant aqueous systems, *Biomass Convers. Biorefine.*, 15(17), 24227-24241(2025). <https://doi.org/10.1007/s13399-024-05534-0>
- Wang, X., Wang, T., Song, C., Zhang, Y., Yang, K., Wang, J., Xu, X. and He, F., Competitive adsorption behavior of As (V) and Sb (V) on Hematite: Facet and pH dependent coordination affinity and role of outer-sphere complexes, *Separat. Purif. Technol.*, 354, 128916(2025). <https://doi.org/10.1016/j.seppur.2024.128916>
- Wen, Y. Z., Xue, Y. Q., Cui, Z. X. and Wang, Y., Thermodynamics of nano-adsorption from solution: theoretical and experimental research, *J. Chem. Thermodyn.*, 80, 112-118(2015). <https://doi.org/10.1016/j.jct.2014.08.013>
- Yao, C., Chen, T., A film-diffusion-based adsorption kinetic equation and its application, *Chem. Eng. Res. Des.*, 119, 87-92(2017). <https://doi.org/10.1016/j.cherd.2017.01.004>
- You, J., Wang, L., Zhao, Y. and Bao, W., A review of amino-functionalized magnetic nanoparticles for water treatment: Features and prospects, *J. Clean. Prod.*, 281, 124668(2021). <https://doi.org/10.1016/j.jclepro.2020.124668>
- Yousaf, Z. and Saleh, N., Advanced concept of green synthesis of metallic nanoparticles by reducing phytochemicals, *Nanobot.*, 17-36(2018). https://doi.org/10.1007/978-3-319-77119-9_2
- Zhang, Y., Zeng, D., Li, L., Hong, X., Li-Byarlay, H. and Luo, S., Assessing the toxicological interaction effects of imidacloprid, thiamethoxam, and chlorpyrifos on *Bombus terrestris* based on the combination index, *Sci. Rep.*, 12(1), 6301(2022). <https://doi.org/10.1038/s41598-022-09808-3>